

Exploring bio-inspired systems:
a synergy between multiscale experimental and
Computational approaches
Wien, September 4, 2024 - September 7, 2024

Guiding colloidal SAT-assembly

The power of patchyness

!

Francesco Sciortino, Sapienza Università' di Roma



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Educated Guess Design

Triblock Janus Particles

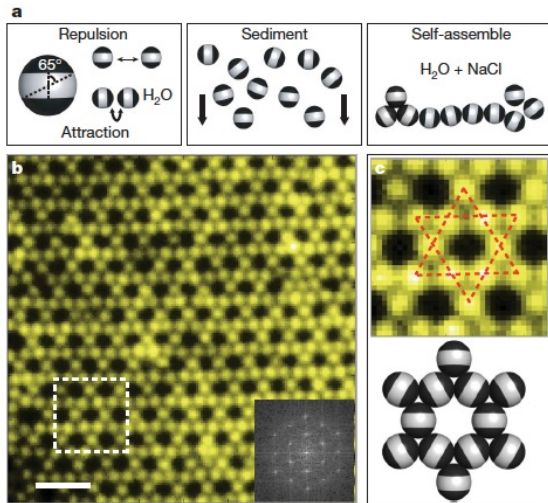
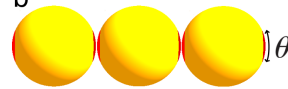
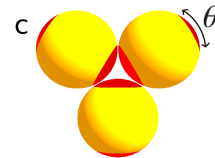


Figure 1 | Colloidal kagome lattice after equilibration. a, Triblock Janus spheres hydrophobic on the poles (black, with an opening angle of 65°) and charged in the equator section (white), are allowed to sediment in deionized water. Then NaCl is added to screen electrostatic repulsion, allowing self-assembly by short-range hydrophobic attraction. b, Fluorescence image of a colloidal kagome lattice (main image) and its fast Fourier transform image (bottom right). Scale bar is $4\ \mu\text{m}$. The top panel in c shows an enlarged view of the dashed white rectangle in b. Dotted red lines in c highlight two staggered triangles. The bottom panel in c shows a schematic illustration of particle orientations.

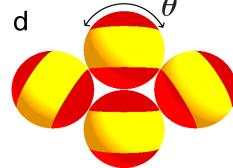
Small patch (chains)



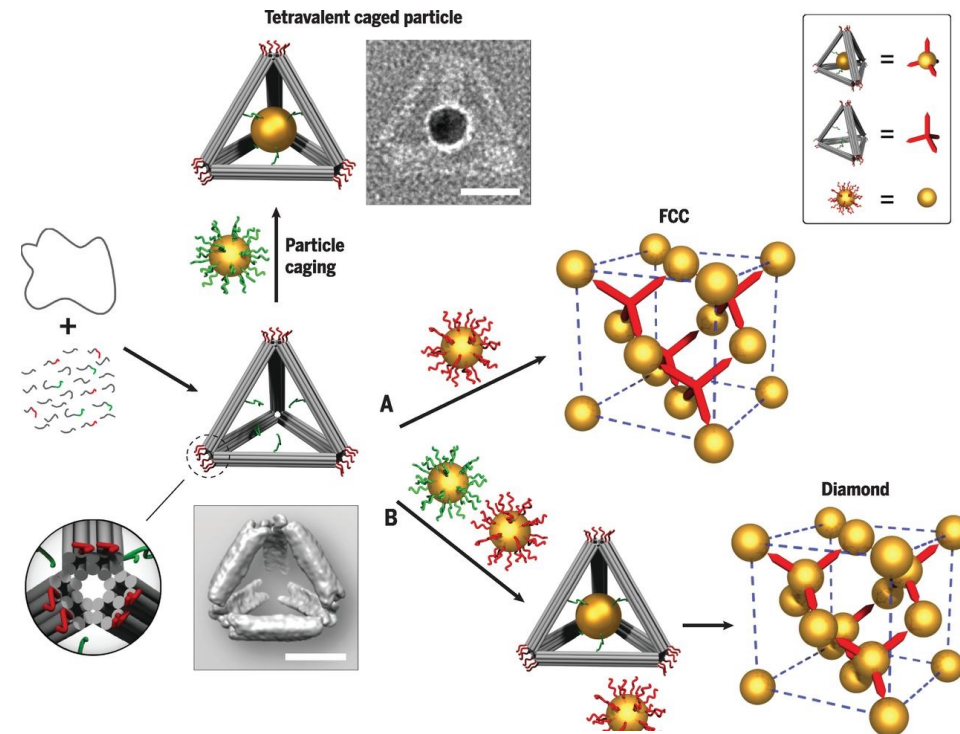
Medium patch (Kagome)



Large patch (dense crystal)



DNA wireframe origami



MATERIALS SCIENCE

Diamond family of nanoparticle superlattices

Wenyan Liu,¹ Miho Tagawa,² Huolin L. Xin,¹ Tong Wang,³ Hamed Emamy,⁴ Huilin Li,^{3,5} Kevin G. Yager,¹ Francis W. Starr,⁴ Alexei V. Tkachenko,¹ Oleg Gang^{1*}

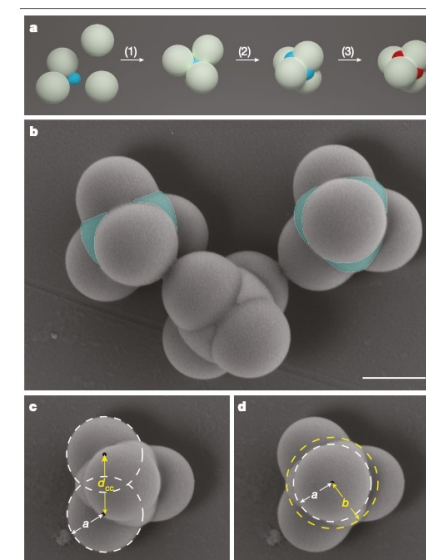
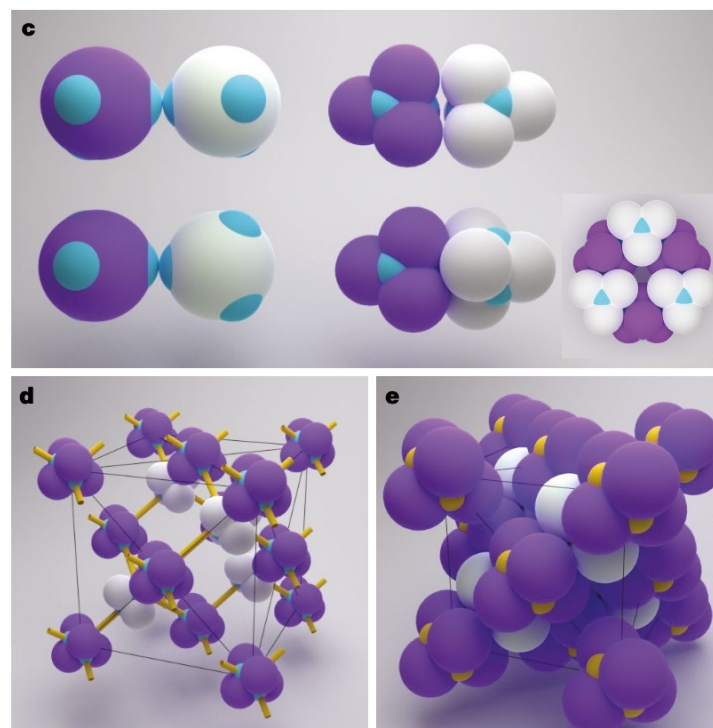
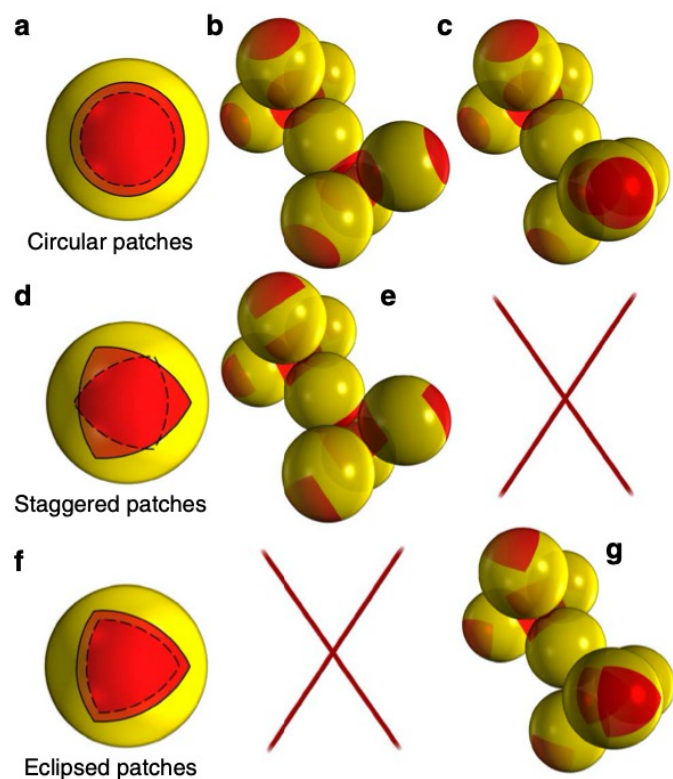
LETTER

doi:10.1038/nature09713

Directed self-assembly of a colloidal kagome lattice

Jian Chen¹, Sung Chul Bae² & Steve Granick^{1,2,3}

Educated Guess Design



ARTICLE

Received 12 Mar 2012 | Accepted 21 Jun 2012 | Published 24 Jul 2012

DOI: 10.1038/ncomms1968

Patterning symmetry in the rational design of colloidal crystals

Flavio Romano^{1,*} & Francesco Sciortino^{2,*}

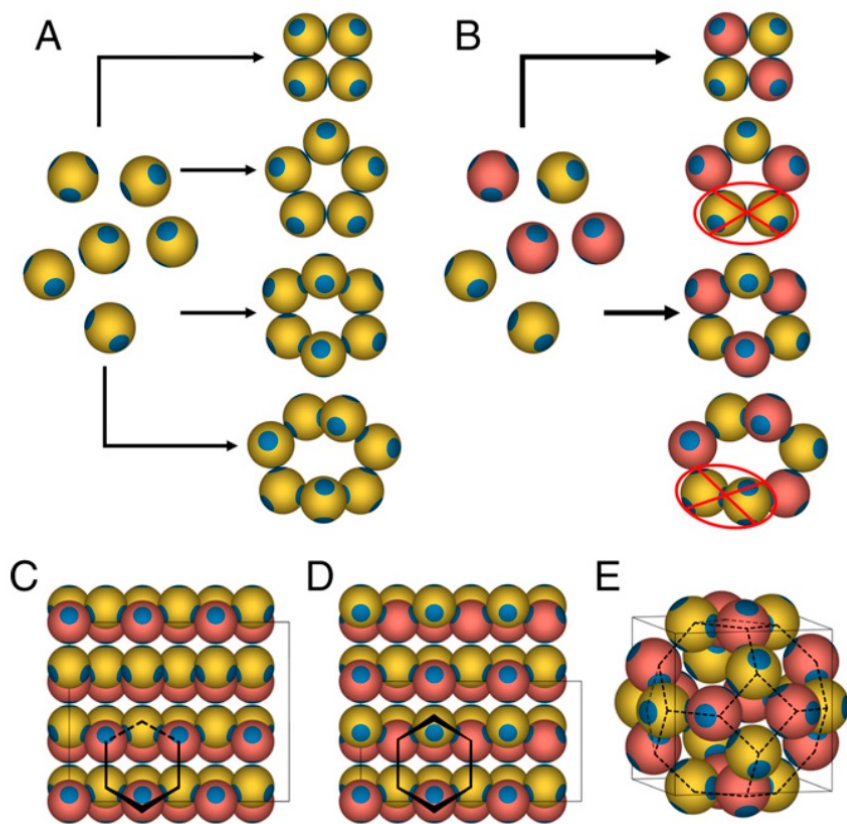
Colloidal diamond

<https://doi.org/10.1038/s41586-020-2718-6>

Received: 9 February 2020

Mingxin He^{1,2}, Johnathon P. Gales², Étienne Ducrot^{2,3}, Zhe Gong⁴, Gi-Ra Yi⁵, Stefano Sacanna^{4,5} & David J. Pine^{1,2,5}

Educated Guess Design



Facile self-assembly of colloidal diamond from tetrahedral patchy particles via ring selection

Andreas Neophytou^a, Dwaipayan Chakrabarti^{a,1}, and Francesco Sciortino^{b,1}

^aSchool of Chemistry, University of Birmingham, Edgbaston, Birmingham B15 2TT, United Kingdom; and ^bDipartimento di Fisica, Sapienza Università di Roma, 00185 Roma, Italy

Potential pitfalls typically encountered in self- assembly

- * metastable states that can compete with the final product;

(cubic diamond, hexagonal diamond, clathrates)



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Potential pitfalls typically encountered in self- assembly

- * metastable states that can compete with the final product;
- * dynamically arrested states (kinetic traps);

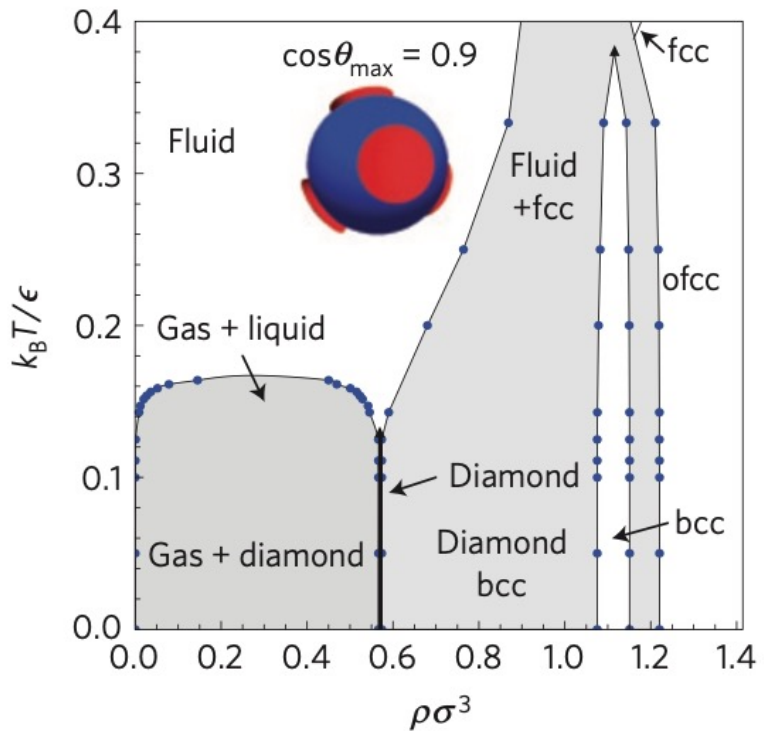
(glasses, gels)



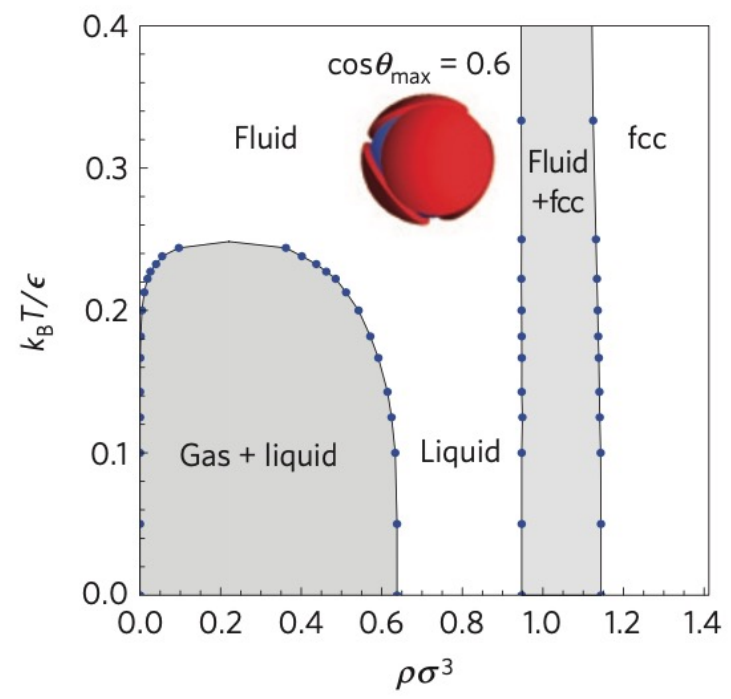
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Tetrahedral patchy particles phase diagram – role of the potential parameters



Directional bonds



Flexible bonds

The *SAT assembly* way

From patchy particles to finite size, periodic and
a-periodic selected structures

The *SAT assembly* way

Use patchy colloidal particles as building blocks

Define as logical variable the lattice and the particle properties

Write the solution in term of CLAUSES which need to be satisfied

Find with a SAT-solver the possible solutions

Designing Patchy Interactions to Self-Assemble Arbitrary Structures

Flavio Romano, John Russo, Lukáš Kroc, and Petr Šulc
Phys. Rev. Lett. **125**, 118003 – Published 10 September 2020

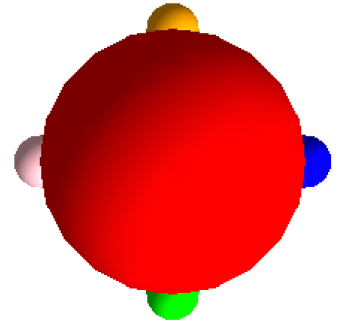
J. Phys.: Condens. Matter **34** (2022) 354002 (11pp)

<https://doi.org/10.1088/1361-6480/ac9002>

SAT-assembly: a new approach for designing self-assembling systems

John Russo^{1,*}, Flavio Romano^{2,3}, Lukáš Kroc⁴, Francesco Sciortino¹,
Lorenzo Rovigatti^{1,5} and Petr Šulc^{4,*}

Why Patchy particles as building blocks ?

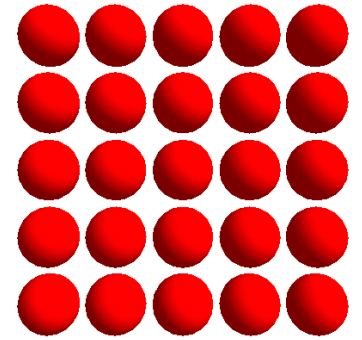


- (i) Can be experimentally realized (colloids, origami)
- (ii) The thermodynamic behaviour of these models is very well understood (Wertheim theory)
- (iii) Computationally efficient (this is required to observe self-assembly phenomena in silico).

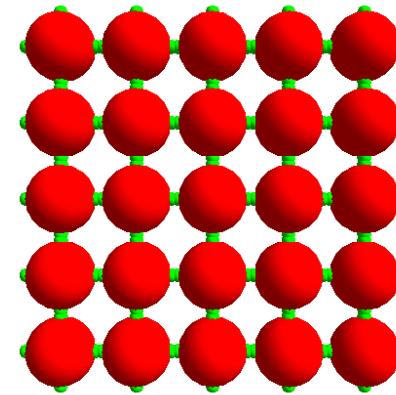


SAT Assembly Steps:

Pick the target (**square**) lattice ($0 < i < L$ lattice sites)

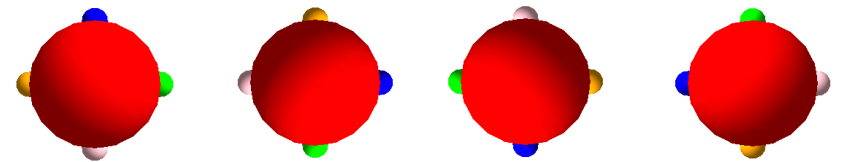


Define the connections (slots) – 4 per particle -- (patchy particles)



Define the number of different patchy particles and the number of different colours (N_p , N_c)

Define orientations



(some of) The logical variables defined to solve the coloring process

$x_{l,p,o}^{Lattice}$ True if lattice site **l** is occupied by particle type **p** with orientation **o**

$x_{p,s,c}^{Patch\ Colour}$ True if patch number **s** of particle **p** has color **c**

$x_{c_i,c_j}^{ColourInteraction}$ True if color **c_i** interact with color **c_j**

$x_{l,s,c}^{DesignVariables}$ True if the slot **s** of lattice site **l** has colour **c**

10⁵ variables

(some) Clauses to solve the coloring process (NOT \neg and OR \vee)

Each site is occupied by only one particle type with specified orientation

$$C_{l,p_i,o_i,p_j,o_j}^L = \bar{x}_{l,p_i,o_i}^{Lattice} \vee \bar{x}_{l,p_j,o_j}^{Lattice}.$$

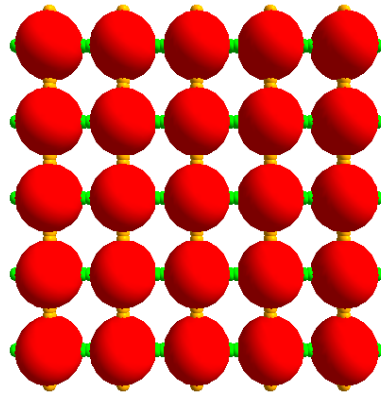
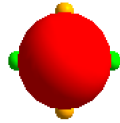
Each color can be complementary to only one other color

$$C_{c_i,c_j,c_k}^{int} = \bar{x}_{c_i,c_j}^{ColourInteraction} \vee \bar{x}_{c_i,c_k}^{ColourInteraction}.$$

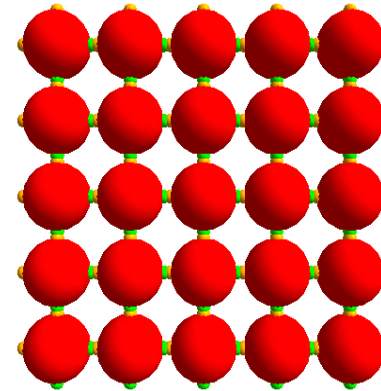
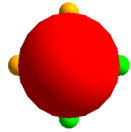
Neighboring positions l_i and l_j connected by slots s_i and s_j must have color c_i and c_j that can bind to each other

Some solutions:

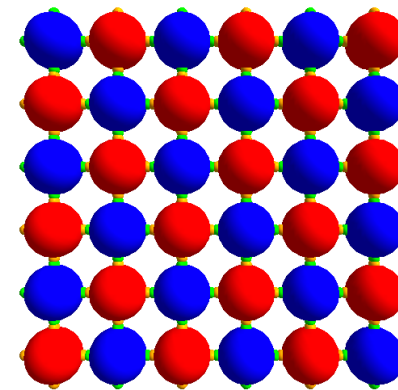
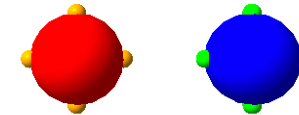
$N_p=1, N_c=2$ G-G,
O-O



$N_p=1, N_c=2$
G-O

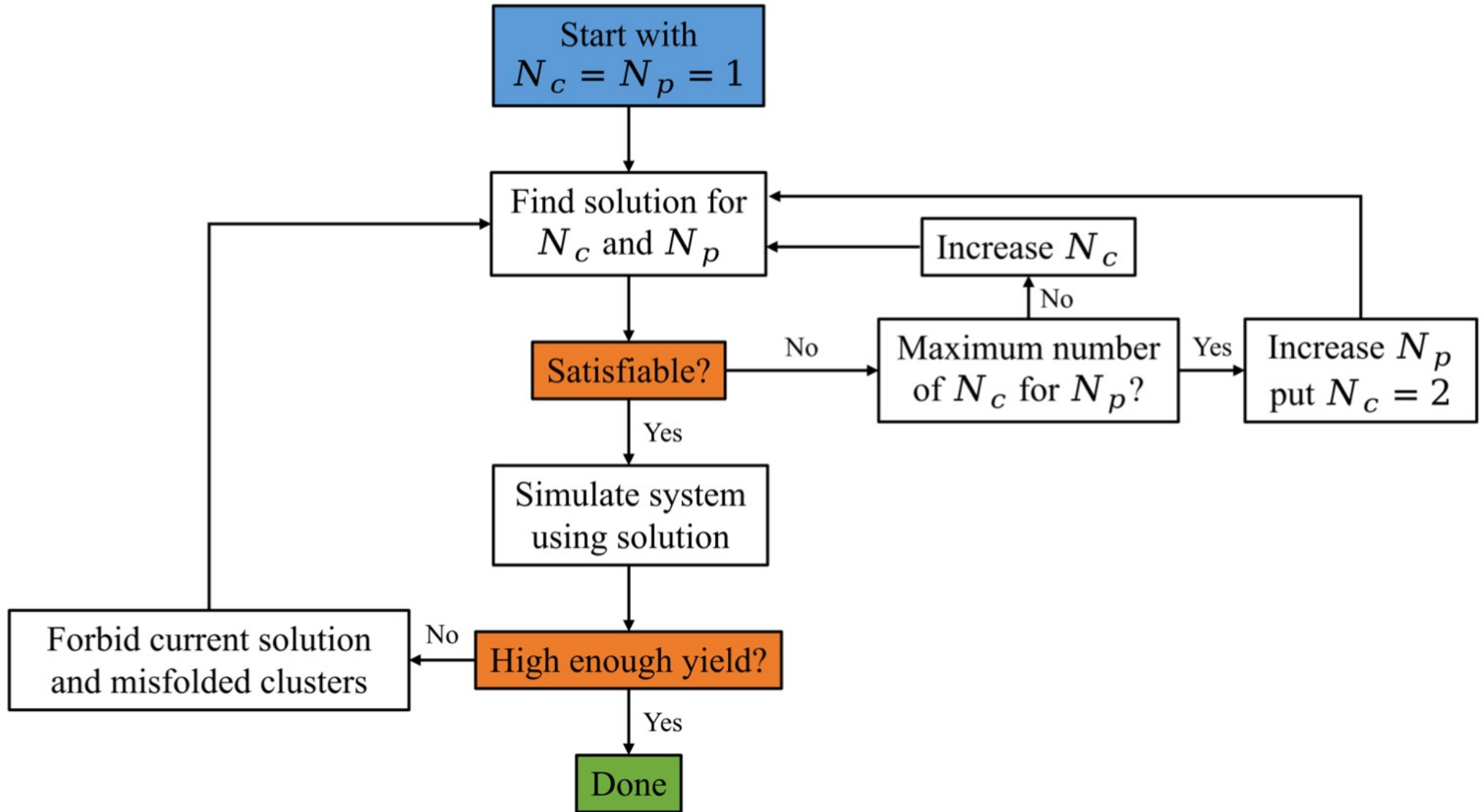


$N_p=2, N_c=2$
G-O



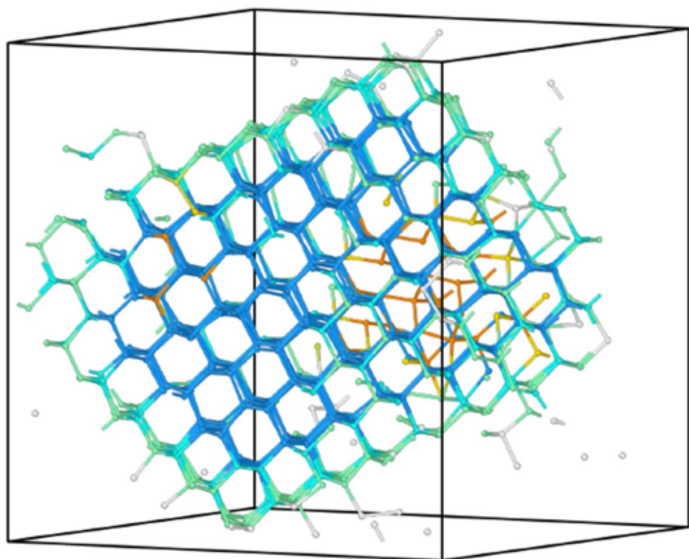
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The SAT-ASSEMBLY pipeline



Cubic (and only cubic) diamond

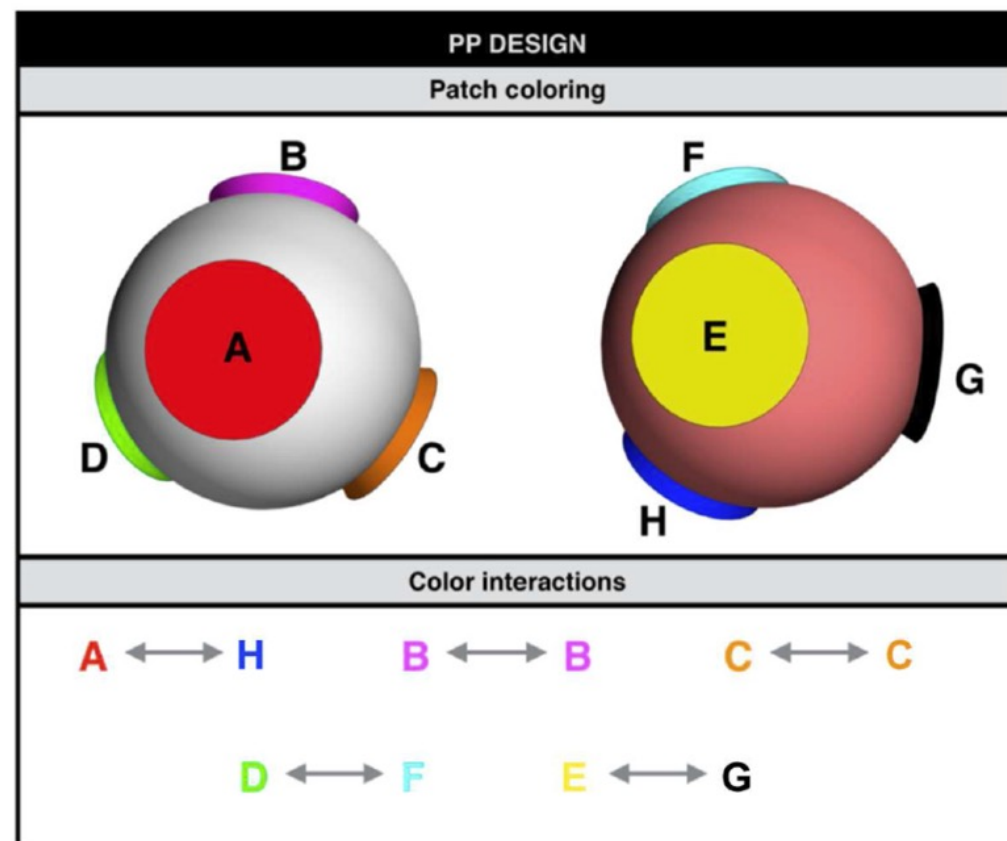
$$N_p=2, N_c=8$$



A simple solution to the problem of
self-assembling cubic diamond
crystals†

[Lorenzo Rovigatti](#), ^{*ab} [John Russo](#), ^{*a} [Flavio Romano](#), ^{cd} [Michael Matthies](#), ^e [Lukáš](#)

[Kroc](#) ^e and [Petr Šulc](#) ^{*e}



Two-step nucleation in a binary mixture
of patchy particles

Cite as: J. Chem. Phys. 158, 154502 (2023); doi: 10.1063/5.0140847
Submitted: 31 December 2022 • Accepted: 24 March 2023 •
Published Online: 17 April 2023

Camilla Beneduce,¹ Diogo E. P. Pinto,¹ Petr Šulc,^{2,3} Francesco Sciortino,¹ and John Russo^{1,a)}

Self Assembly in Multi component systems....

Gas \rightarrow Liquid \rightarrow Crystal

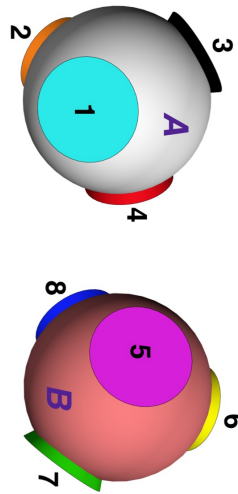
Consumption of the minority component

Azeotropy: when a multicomponent system behaves as a one component one

When coexisting phases have the same

$$N_p=2, N_c=8$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$



$$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{pmatrix}$$

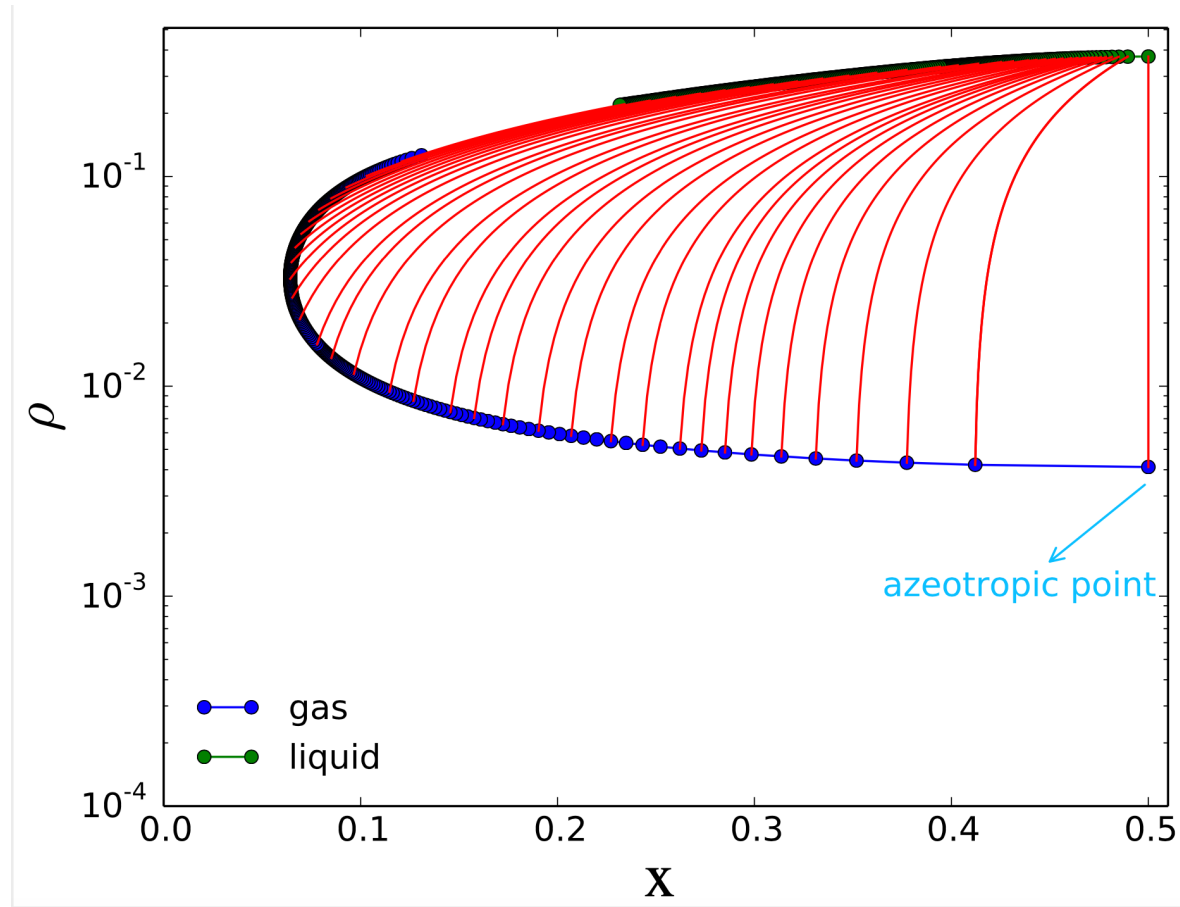
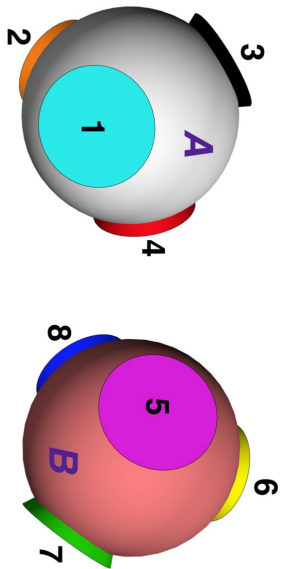
One 1 in each row
(*azeotropic at equimolar*)

Two 1 in each row
(but on different
particles, *azeotropic at
all compositions*)

Why and How to include azeotropy in the design of self-assembling systems

Camilla Beneduce,¹ Francesco Sciortino,¹ Petr Šulc,² and John Russo¹

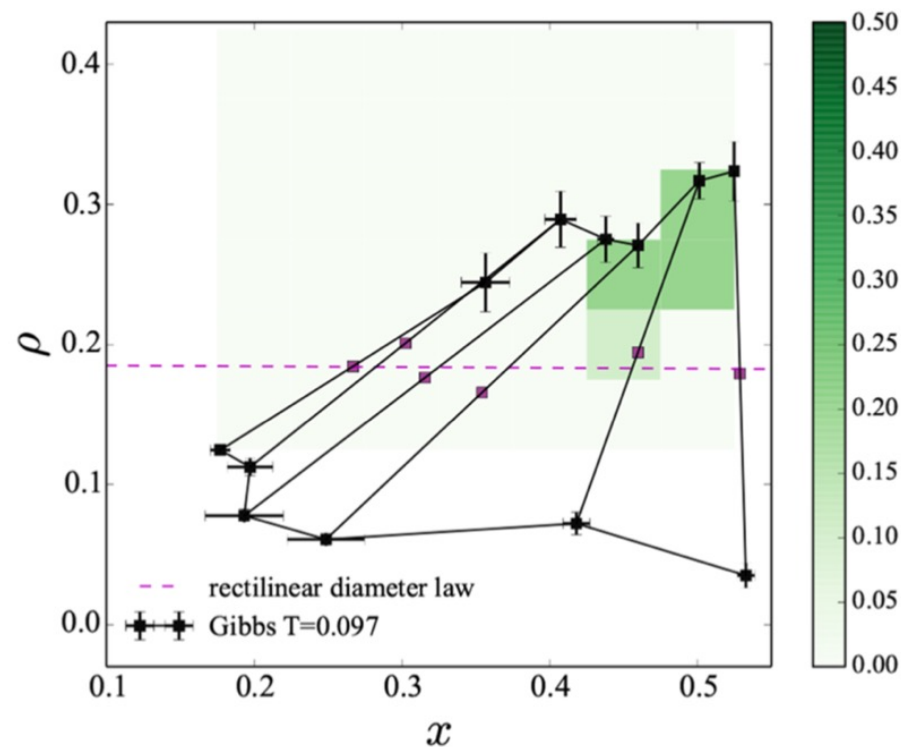
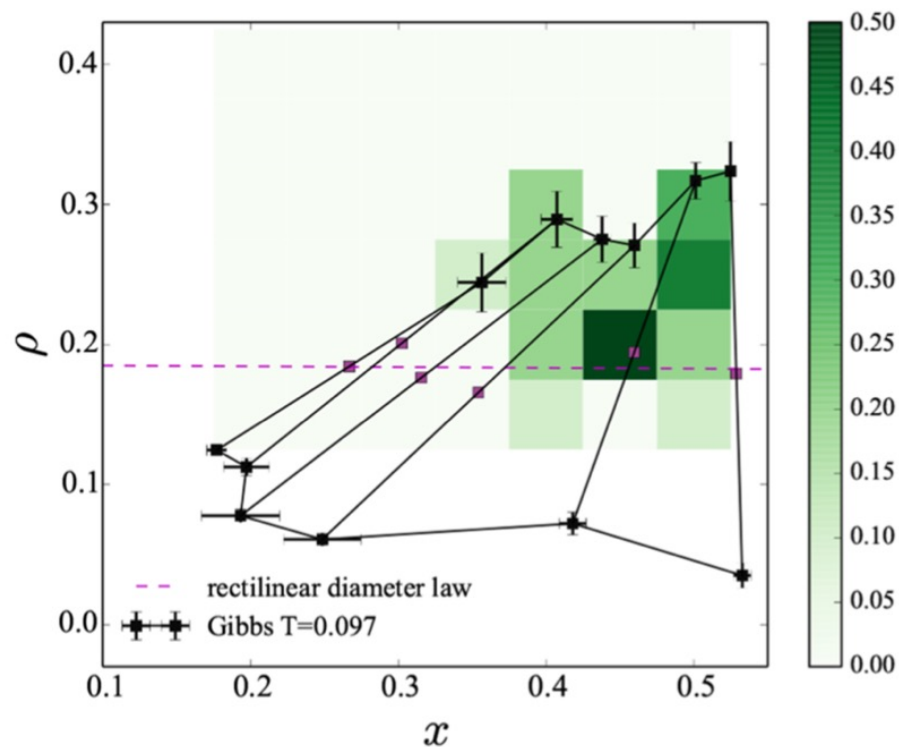
*Theoretical predictions based on Wertheim theory
(case: azeotropic at equimolar)*



Why and How to include azeotropy in the design of self-assembling systems

Camilla Beneduce,¹ Francesco Sciortino,¹ Petr Šulc,² and John Russo¹

Numerical results: Azeotropy favours nucleation !



Two-step nucleation in a binary mixture of patchy particles

Cite as: J. Chem. Phys. 158, 154502 (2023); doi: [10.1063/5.0140847](https://doi.org/10.1063/5.0140847)

Submitted: 31 December 2022 • Accepted: 24 March 2023 •

Published Online: 17 April 2023



Camilla Beneduce,¹  Diogo E. P. Pinto,¹  Petr Šulc,^{2,3}  Francesco Sciortino,¹  and John Russo^{1,a)} 

Finite size clusters

Archimedean polyhedral shells that can be assembled from building blocks with a coordination number of five:

the 12-particle *icosahedron*,



the 24-particle *snub cube*,

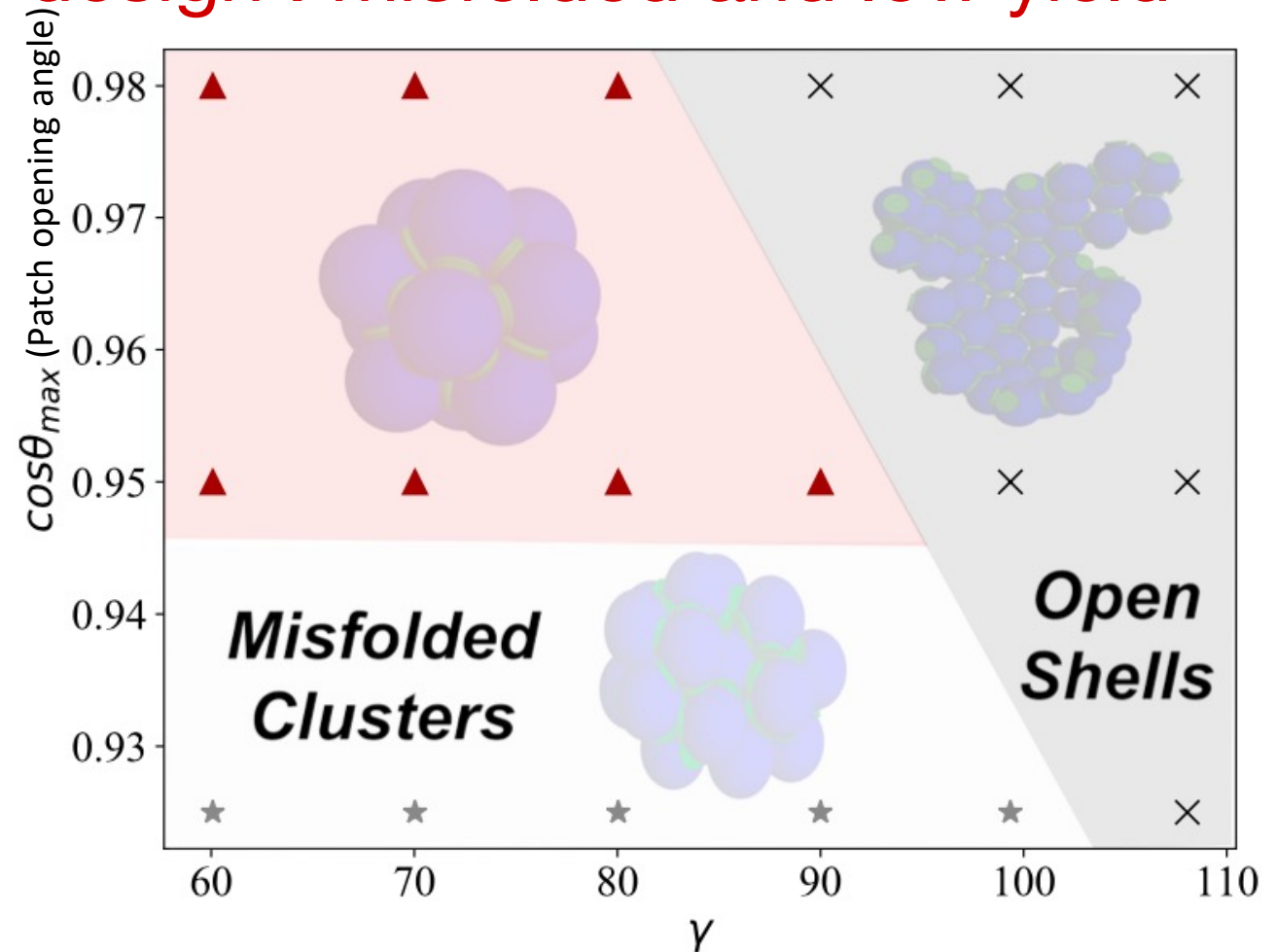
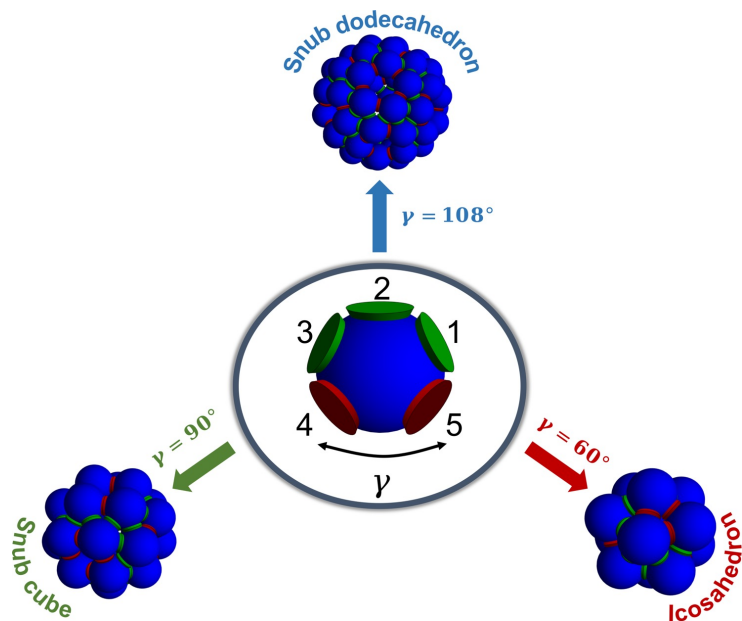


the 60-particle *snub dodecahedron*.



The educated guess design : misfolded and low yield

$$N_c=1 \quad N_p=1$$



(angle between patch 4 and 5 – see figure)

PNAS

RESEARCH ARTICLE | PHYSICS

Design strategies for the self-assembly of polyhedral shells

Diogo E. P. Pinto^a, Petr Šulc^{b,c}, Francesco Sciortino^a, and John Russo^{a,1}

$N_p=1, N_c=2, 3, 4, 5$: Colouring improves:

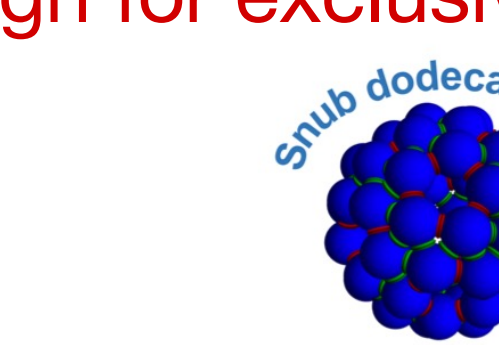
Solution	C2(1)	C2(2)	C3(1)	C3(2)	C4(1)	C4(2)	C5
Design							
Interaction	$A \leftrightarrow A$ $B \leftrightarrow B$	$A \leftrightarrow A$ $B \leftrightarrow B$	$A \leftrightarrow A$ $B \leftrightarrow C$	$A \leftrightarrow A$ $B \leftrightarrow B$ $C \leftrightarrow C$	$A \leftrightarrow D$ $B \leftrightarrow B$ $C \leftrightarrow C$	$A \leftrightarrow D$ $B \leftrightarrow B$ $C \leftrightarrow C$	$A \leftrightarrow A$ $B \leftrightarrow C$ $D \leftrightarrow E$

Increasing the Number of Colours Increases the Yield.

Decreasing the Symmetry of the Building Block Increases the Yield.

Finite size clusters

Minimum Design for exclusive assembly



Solution	Icosahedron		Snub cube		Snub dodecahedron			
Design								
Interaction	$N_c=5$ $ \begin{aligned} &F \leftrightarrow F \\ &B \leftrightarrow C \\ &A \leftrightarrow D \end{aligned} $		$N_c=5$ $ \begin{aligned} &F \leftrightarrow F \\ &B \leftrightarrow C \\ &A \leftrightarrow D \end{aligned} $		$N_c=11$ $ \begin{aligned} &A \leftrightarrow F \\ &G \leftrightarrow H \\ &I \leftrightarrow J \\ &K \leftrightarrow K \\ &D \leftrightarrow D \\ &B \leftrightarrow C \\ &E \leftrightarrow L \end{aligned} $			

Design strategies for the self-assembly of polyhedral shells

Diogo E. P. Pinto^a, Petr Šulc^{b,c} , Francesco Sciortino^a , and John Russo^{a,1}

SAT-assembly and the experiments....

A complete pipeline

Tetrastack:

SAT-assembly and the experiments....

Tetrastack: $N_p=4$, $N_c=24$ (Maximum number of colors)



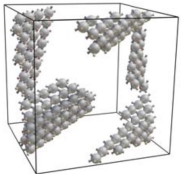
PHOTONIC BANDGAPS

Inverse design of a pyrochlore lattice of DNA origami through model-driven experiments

Hao Liu¹, Michael Matthies¹, John Russo², Lorenzo Rovigatti², Raghu Pradeep Narayanan^{1,3},
Thong Diep¹, Daniel McKeen⁴, Oleg Gang^{4,5,6}, Nicholas Stephanopoulos¹, Francesco Sciortino²,
Hao Yan¹, Flavio Romano^{7,8}, Petr Šulc^{1,9*}

Liu *et al.*, *Science* **384**, 776–781 (2024)

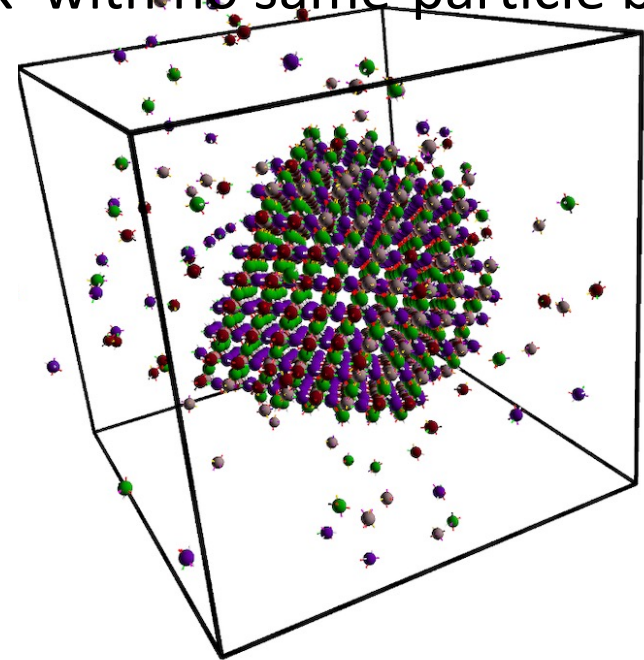
17 May 2024



$N_p=1$ (kinetic traps, alternative structure)

$N_p=2$ OK but with same-particle bonds

$N_p=4$ OK with no same-particle bonds



SAT-assembly and the experiments....

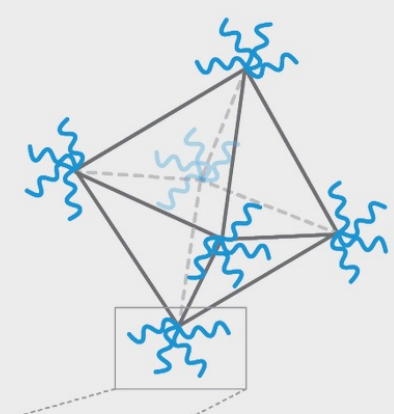
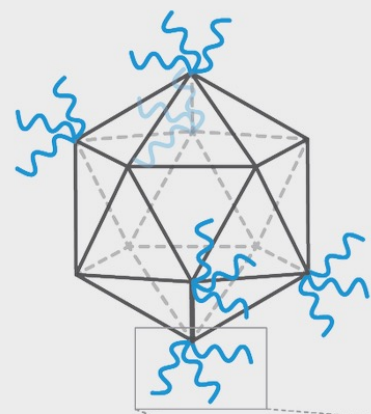
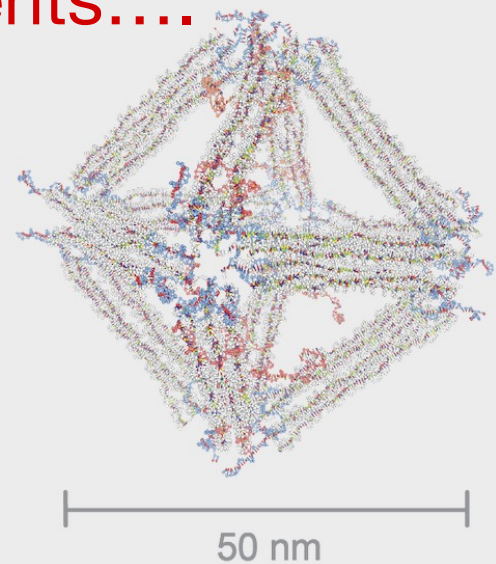
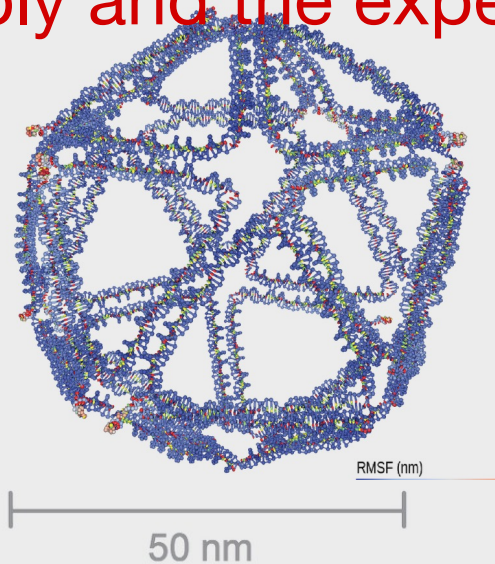
Octahedral

A



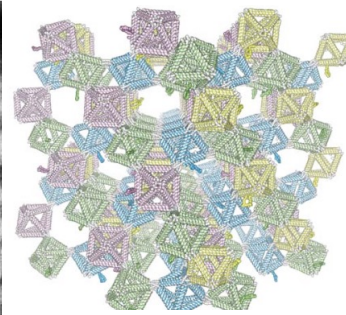
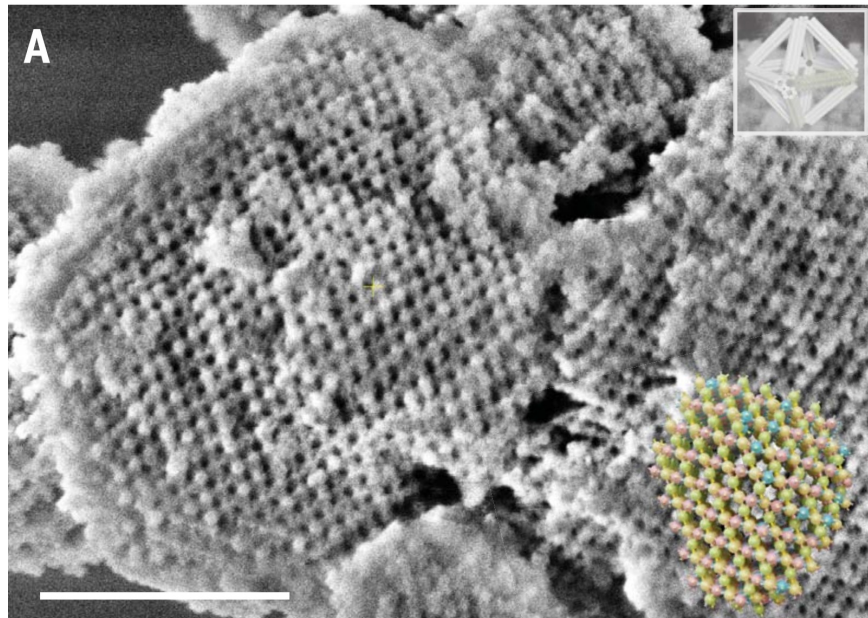
icosahedral

C



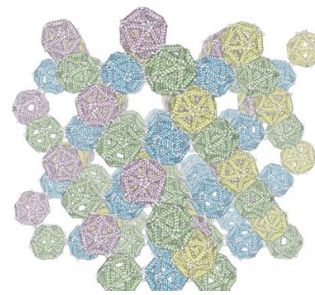
Poly-T spacer Sticky end

Tetrastack

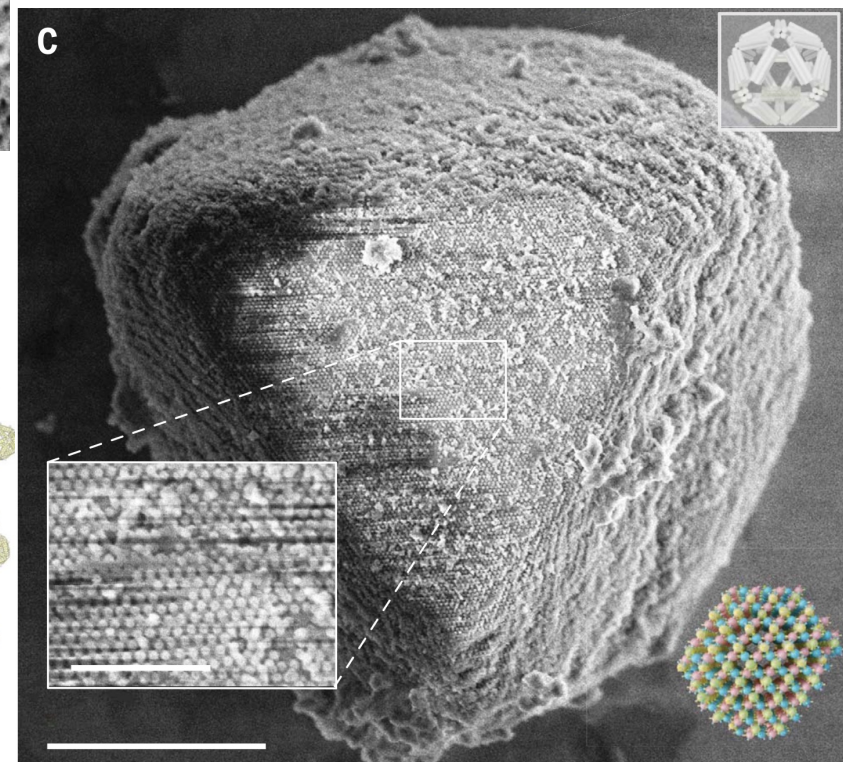


Octahedral

Silica-coated
SEM images

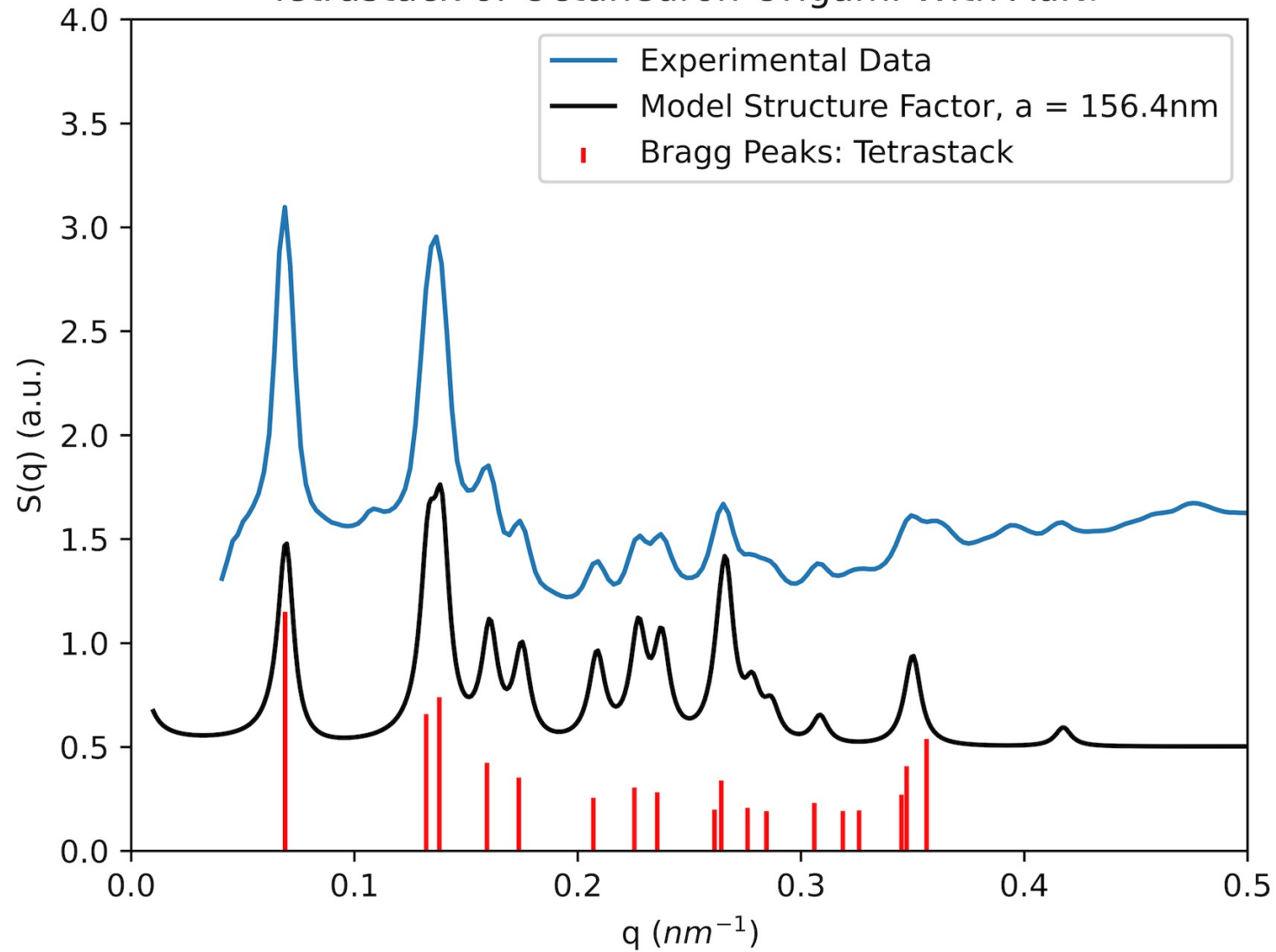


icosahedral



Micron-scale

Tetrastack of Octahedron Origami With AuNP



How to design an icosahedral quasicrystal through directional bonding

<https://doi.org/10.1038/s41586-021-03700-2>

Eva G. Noya^{1,✉}, Chak Kui Wong², Pablo Llombart¹ & Jonathan P. K. Doye^{2,1}

Received: 13 August 2020

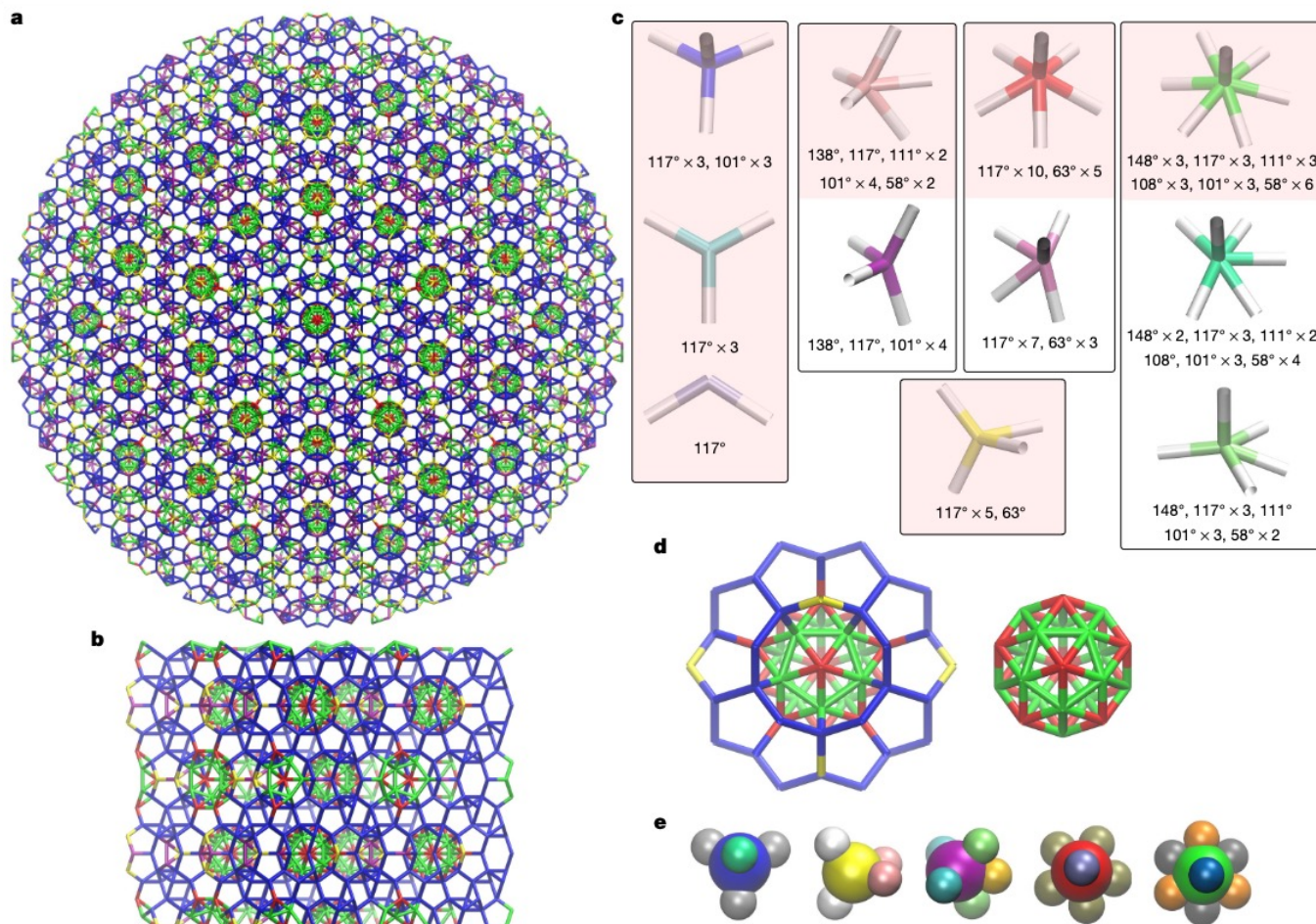
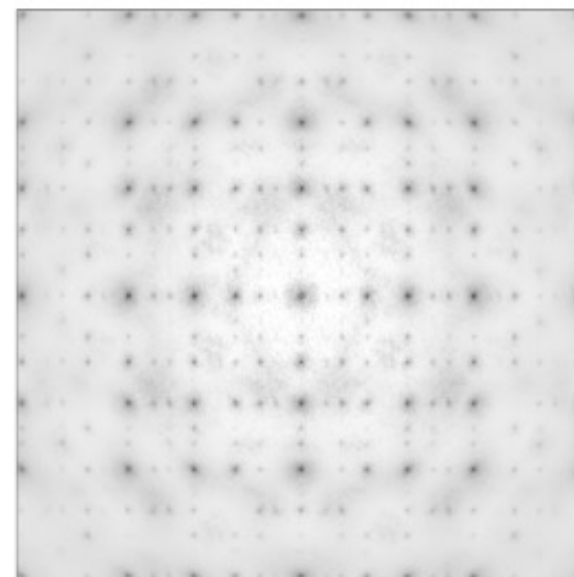
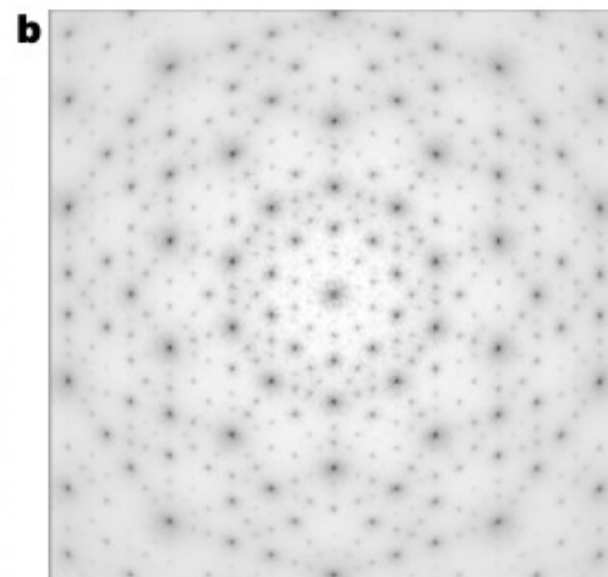
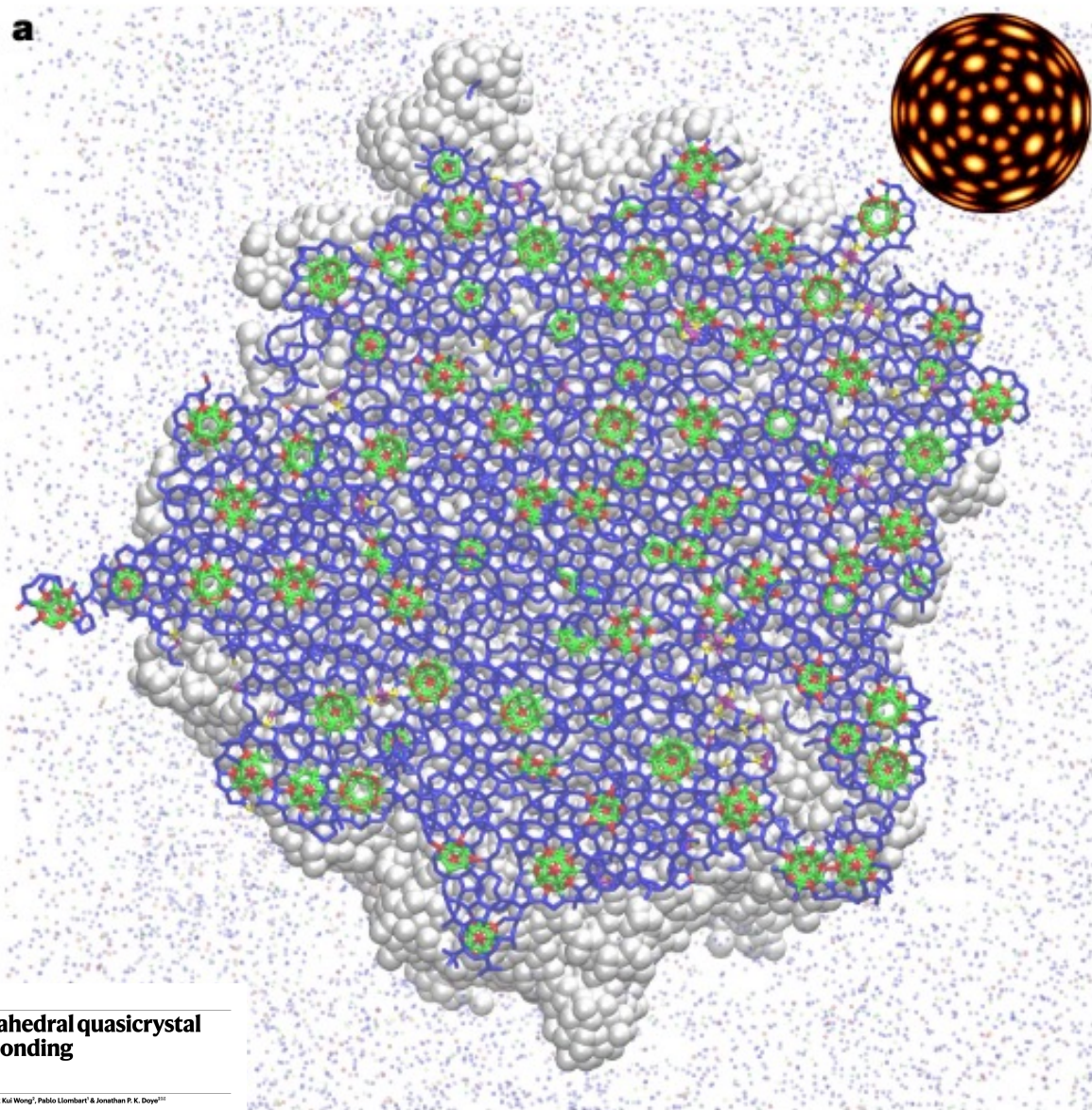


Fig. 1 | From ideal quasicrystal to patchy-particle design. a, Target ideal body-centred IQC structure. **b**, The corresponding 3/2 rational approximant (obtained by the cut-and-project method). **c**, Geometry of the local environments in the ideal quasicrystal organized in classes that are characterized by the same local geometry but with some dangling bonds.

Those local environments also present in the 3/2 rational approximant are shaded in red. **d**, Structure of the icosahedral clusters forming the IQC. The inner shell is a 32-particle triacontahedra, which is surrounded by a shell of 50 four-patch particles. **e**, Model patchy particles used for the assembly of the body-centred SPIQC.



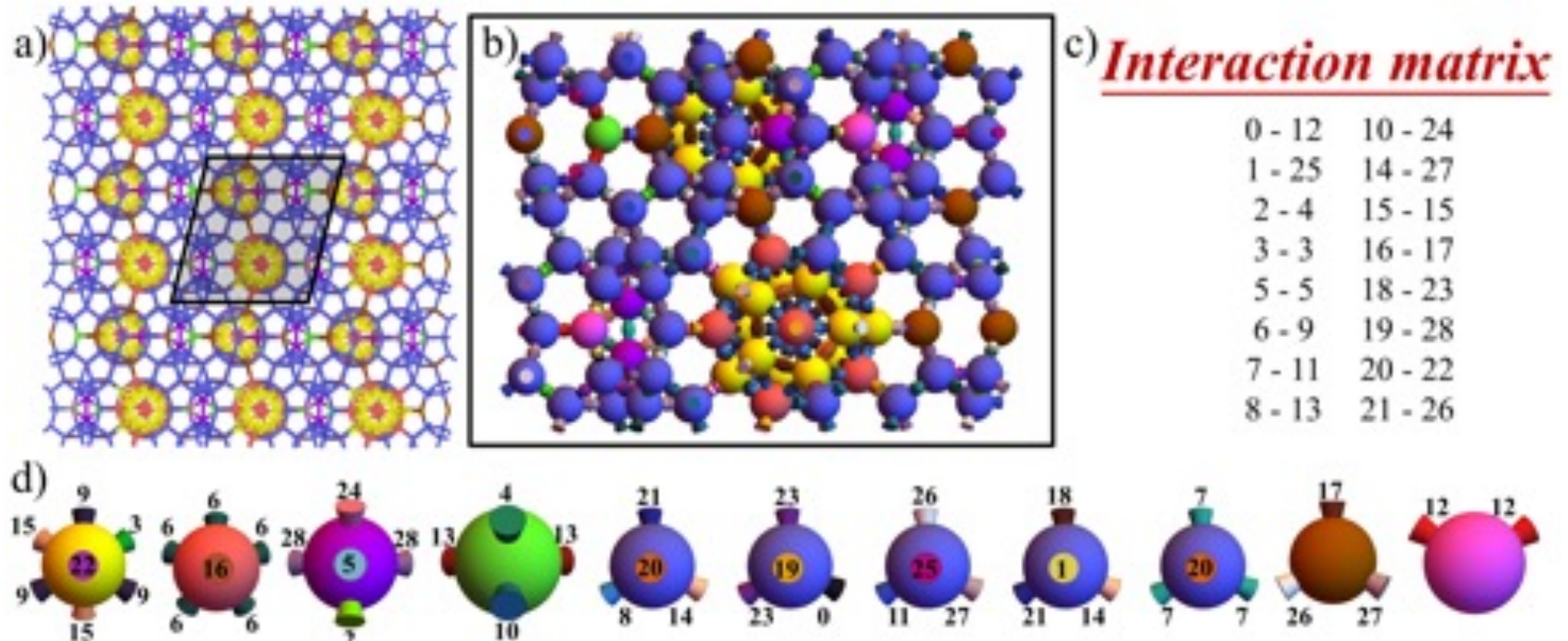
Article

How to design an icosahedral quasicrystal through directional bonding

<https://doi.org/10.1038/s41586-021-03700-2> Eva G. Noya^{1,2}, Chak Kai Wong¹, Pablo Lombart¹ & Jonathan P. K. Doye^{1,2}

Published: 15 August 2021

Proof of concept: Can SAT-assembly solve the problems with colours instead of torsion ?



arXiv > cond-mat > arXiv:2407.19968

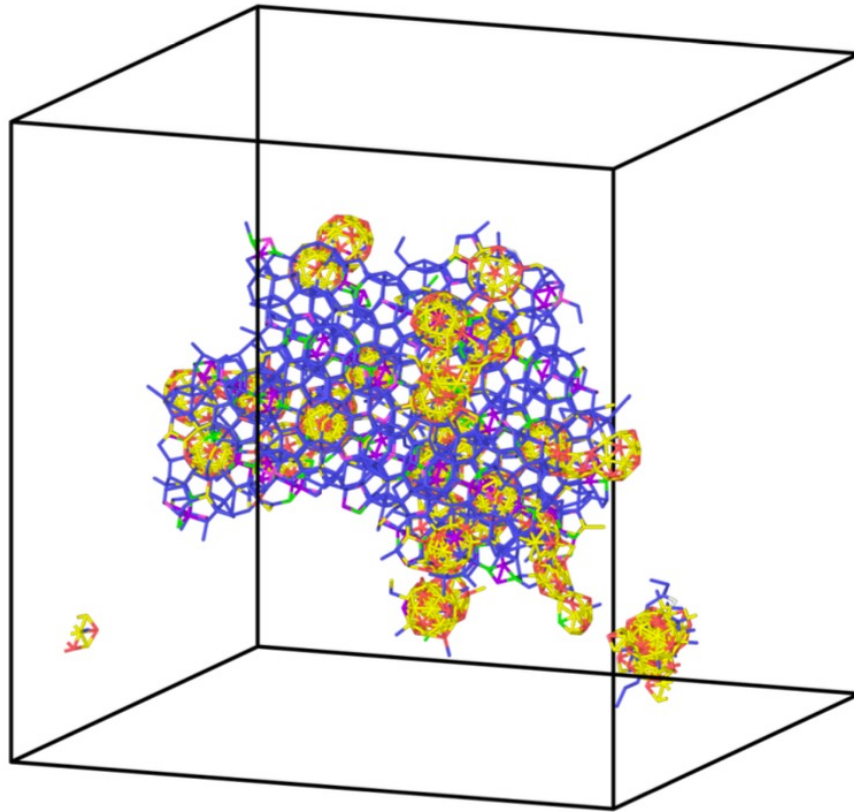
Condensed Matter > Soft Condensed Matter

[Submitted on 29 Jul 2024]

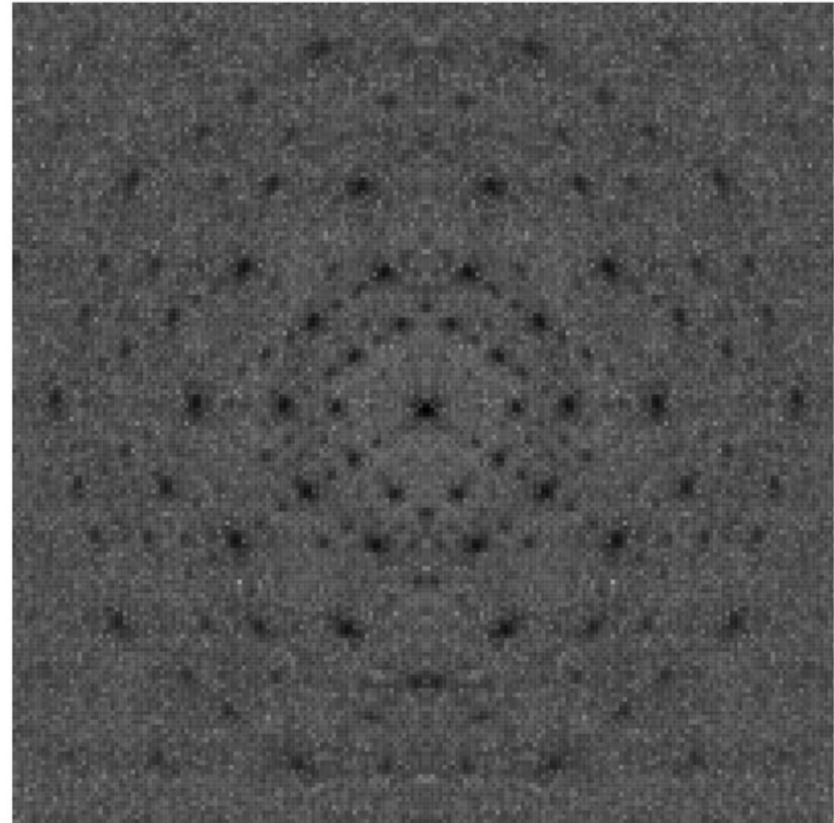
Automating Blueprints for Colloidal Quasicrystal Assembly

Diogo E. P. Pinto, Petr Šulc, Francesco Sciortino, John Russo

Spontaneous formation of the approximant



$$N_p=11 \quad N_c=29$$



arXiv > cond-mat > arXiv:2407.19968

Condensed Matter > Soft Condensed Matter

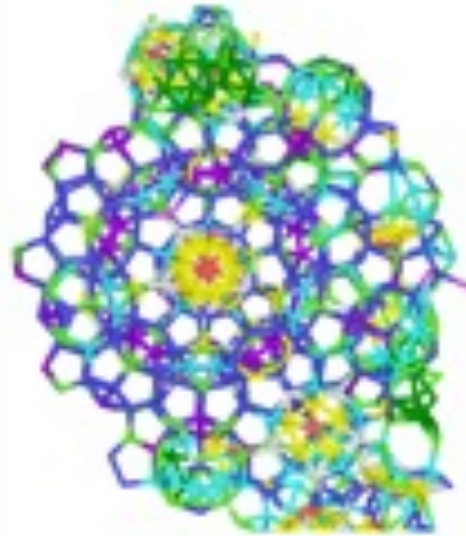
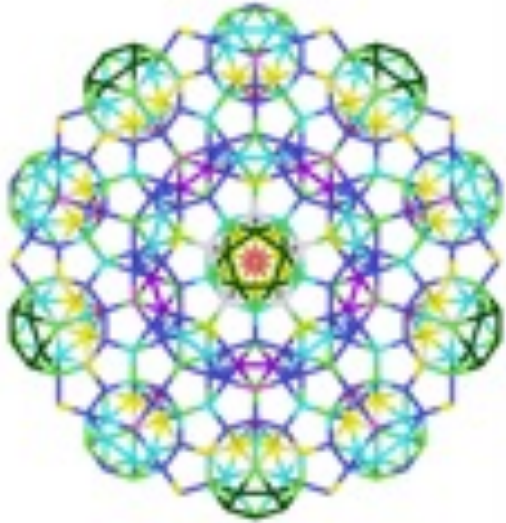
[Submitted on 29 Jul 2024]

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Ideal

Simulation



portion of an ideal
quasicrystal with
 $N = 1538$

$N_p=28$ $N_c=27$

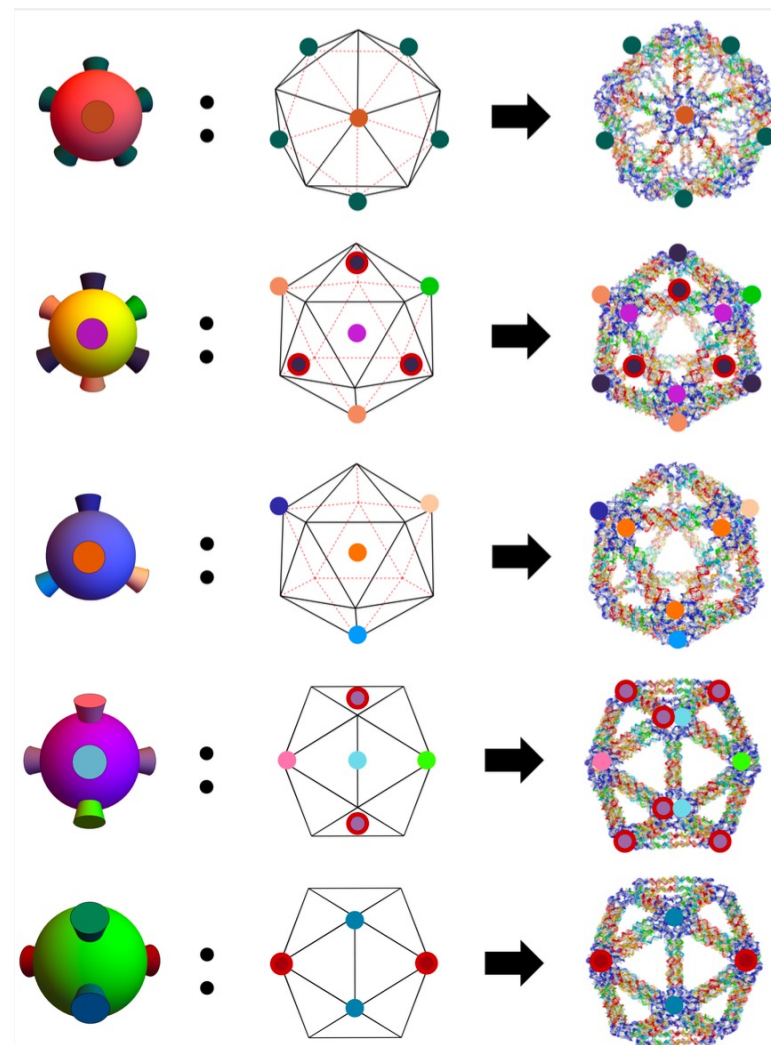
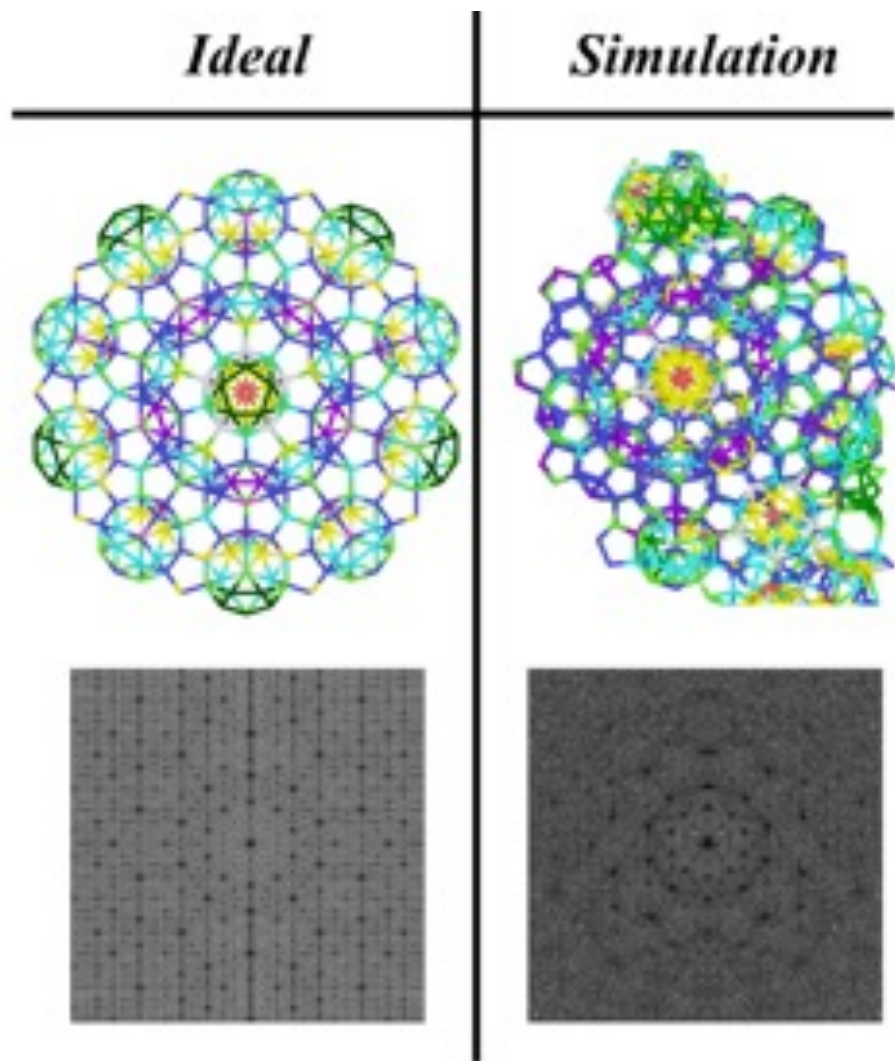
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Take home messages

SAT-Assembly appears to be a valuable method to solve the self-assembly process based on patchy particle's building blocks

Ability to eliminate solutions presenting kinetic traps
Or ending in competing structures
Or encoding experimental requests

Possibility to encode the results into DNA-origami wireframe particles

Take home messages

More colors, easier self-assembly

Less symmetry, easier self-assembly

Azeotropic composition, easier self-assembly

Take home messages

More colors, easier self-assembly

Less symmetry, easier self-assembly

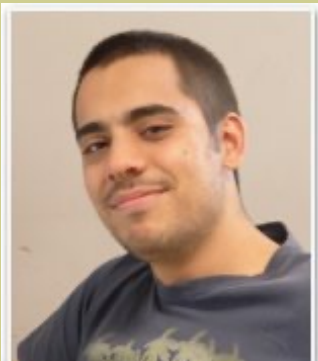
Azeotropic composition, easier self-assembly

THANKS FOR LISTENING !

John Russo



Diogo Pinto



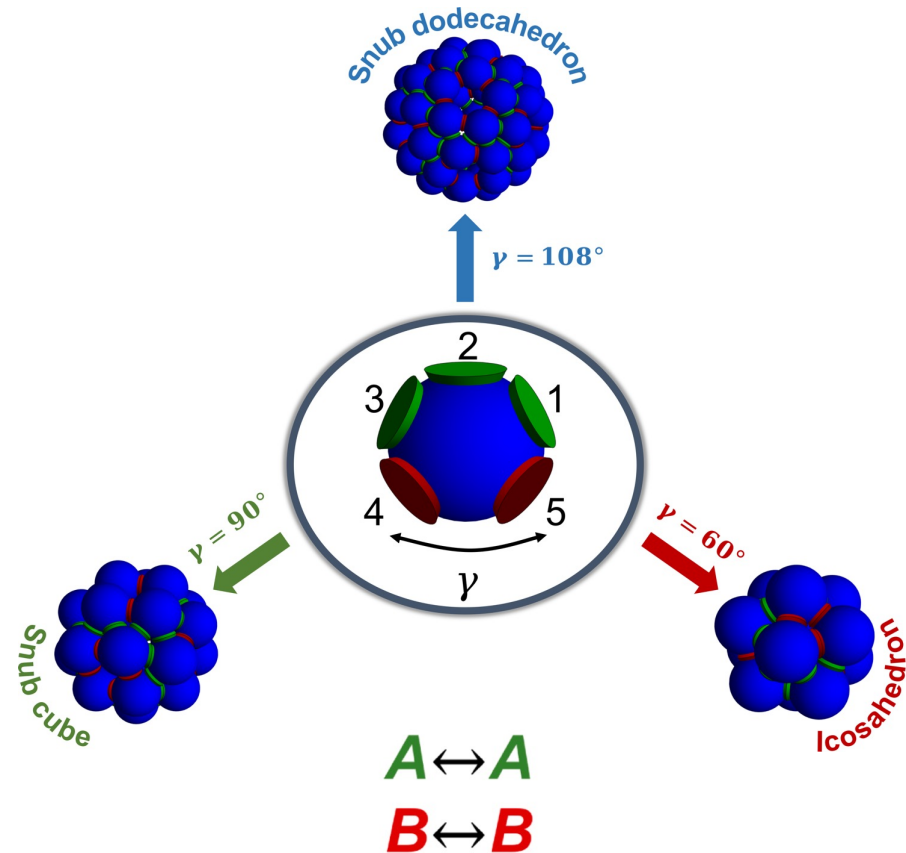
Lorenzo Rovigatti



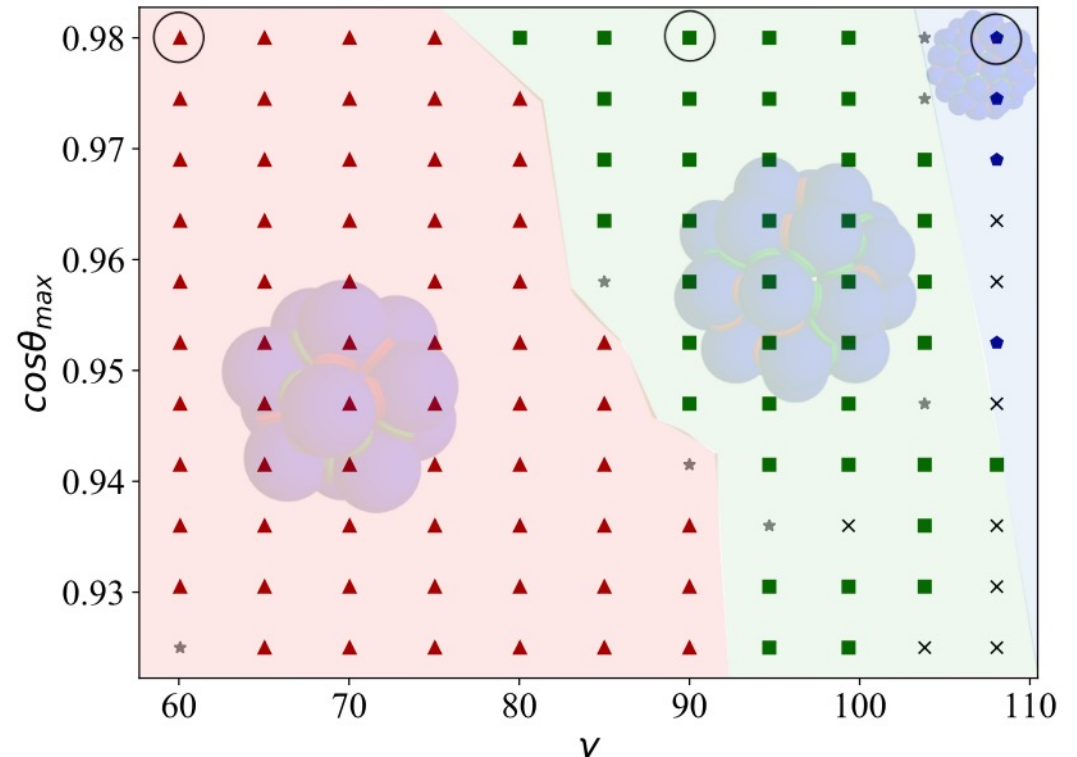
Camilla Beneduce



Pets Sulc



Colouring improves: $N_p=1, N_c=2$



Higher yield, no misfolded, competing structures.

Sufficient condition for azeotropy $X_{\alpha}^{(i)} = X$

- the *bond exclusivity* condition. This rule generates azeotropic points at equimolar conditions;
- the *bond multiplicity* condition. This rule allows for azeotropic points at non-equimolar conditions;
- the *fully-connected bond* condition. This rule generates always-azeotropic mixtures, e.g. where the concentration remains the same during demixing for every point in the coexistence region.

Why and How to include azeotropy in the design of self-assembling systems

Camilla Beneduce,¹ Francesco Sciortino,¹ Petr Šulc,² and John Russo¹

bond exclusivity

each patch has only one bonding partner (that can be itself in case of self-complementarity) among all patches of all species in the mixture.

Azeotropic at equal molar conditions

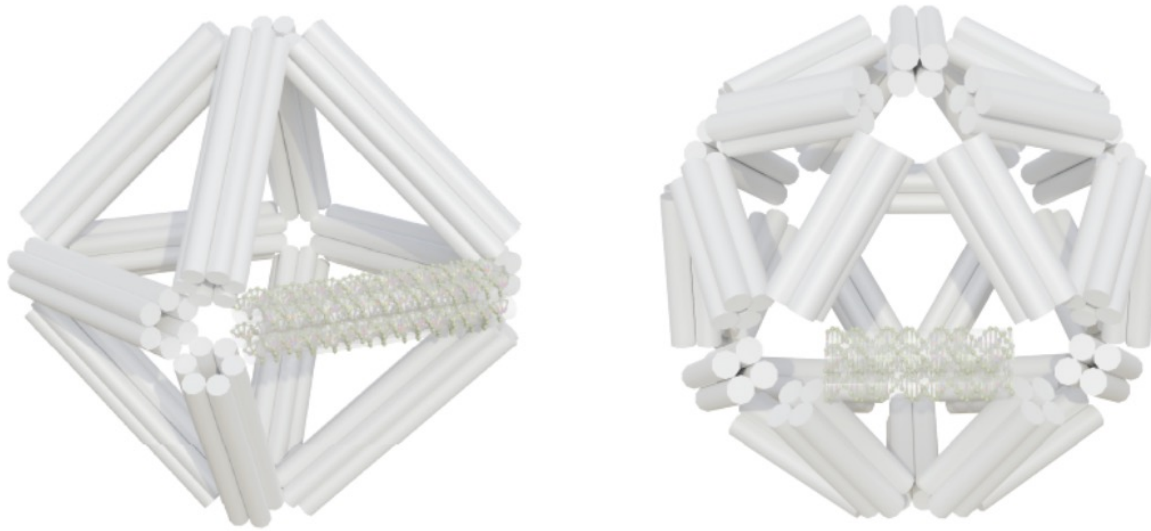
fully-connected bond

each patch can bind with N_s patches, each located on a different species.

Azeotropic at all molar conditions

SAT-assembly and the experiments....

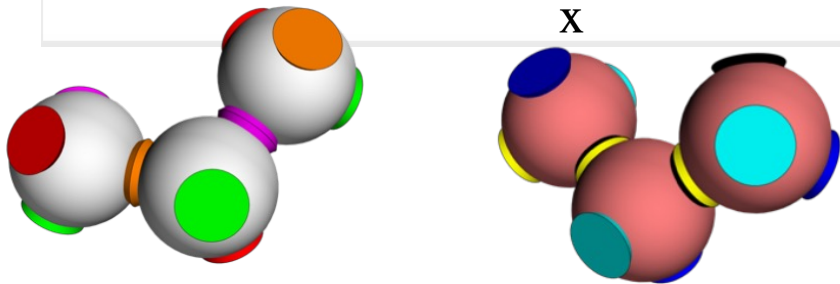
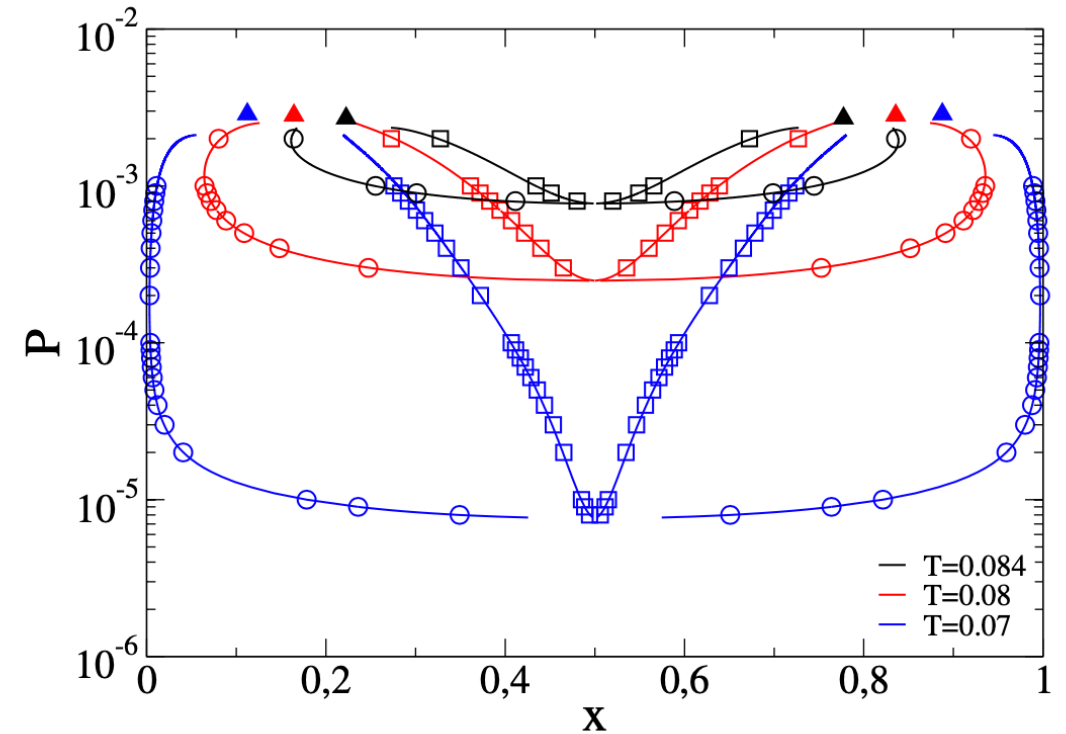
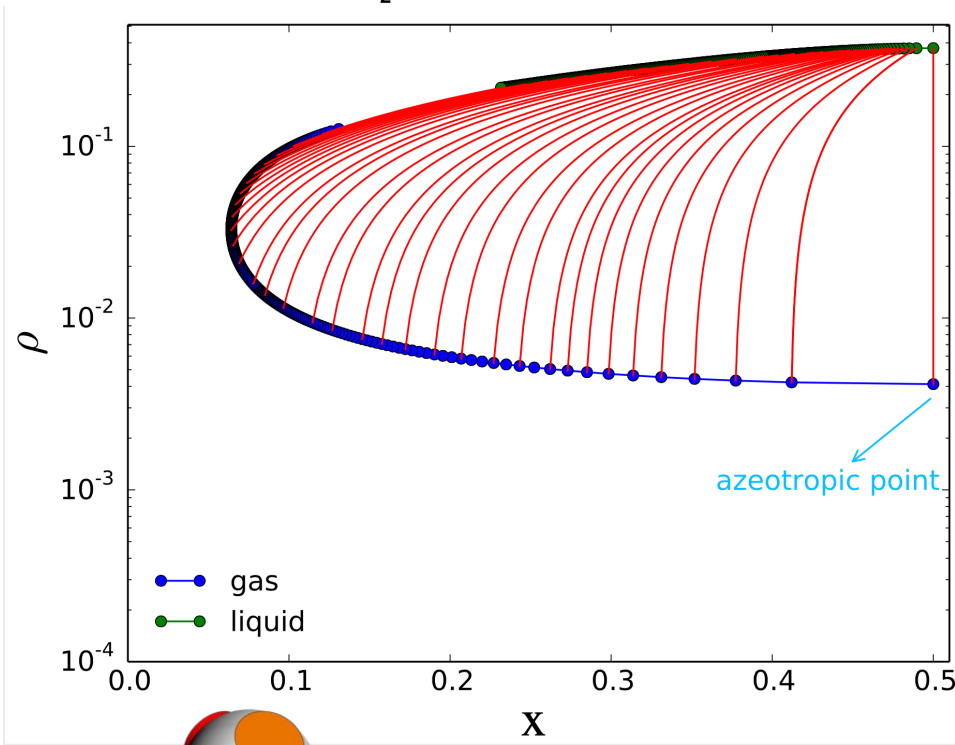
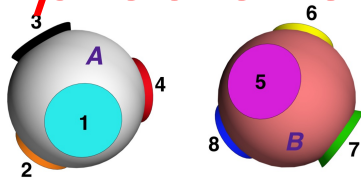
Tetrastack: $N_p=4$, $N_c=24$ (Maximum number)



From model-driven design to experimental realization of tetrastack lattice with DNA nanotechnology

Hao Liu,¹ Michael Matthies,¹ John Russo,² Lorenzo Rovigatti,² Raghu Pradeep Narayanan,¹ Daniel McKeen,³
Oleg Gang,³ Nicholas Stephanopoulos,¹ Francesco Sciortino,² Hao Yan,¹ Flavio Romano,⁴ and Petr Šulc¹

Theoretical predictions based on Wertheim theory (case: azeotropic at equimolar)



Why and How to include azeotropy in the design of self-assembling systems

Camilla Beneduce,¹ Francesco Sciortino,¹ Petr Šulc,² and John Russo¹

Potential pitfalls typically encountered in self- assembly

- * metastable states that can compete with the final product;
- * dynamically arrested states (kinetic traps);
- * low aggregation rates;
- * lack of knowledge of the underlying phase behaviour of the building-blocks, especially for mixtures with many components.



From an experimental point-of-view one need to consider:

- * the difficulty in realizing bulk quantities of building blocks, their size (gravitational effect)
- * the interaction polydispersity (promoting disordered arrest)
- * The difficulty in controlling mechanical and molecular properties, such as softness and flexibility.



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Turning statistical physics models into materials design engines

Marc Z. Miskin^{a,1}, Gurdaman Khaira^b, Juan J. de Pablo^{b,c}, and Heinrich M. Jaeger^a

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Cite This: *J. Phys. Chem. B* 2018, 122, 8462–8468

Inverse Design of Colloidal Crystals via Optimized Patchy Interactions

D. Chen,[†] G. Zhang,[†] and S. Torquato^{*,†,‡,§,||,Ⓜ}

SCIENCE ADVANCES | RESEARCH ARTICLE

MATERIALS SCIENCE

Inverse design of soft materials via a deep learning–based evolutionary strategy

Gabriele M. Coli^{*,†}, Emanuele Boattini^{*,†}, Laura Fillion, Marjolein Dijkstra

Theoretical Approaches

PHYSICAL REVIEW E **98**, 032611 (2018)

Programmable self-assembly of diamond polymorphs from chromatic patchy particles

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²Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York 11973, USA

Annual Review of Chemical and Biomolecular Engineering

Machine Learning–Assisted Design of Material Properties

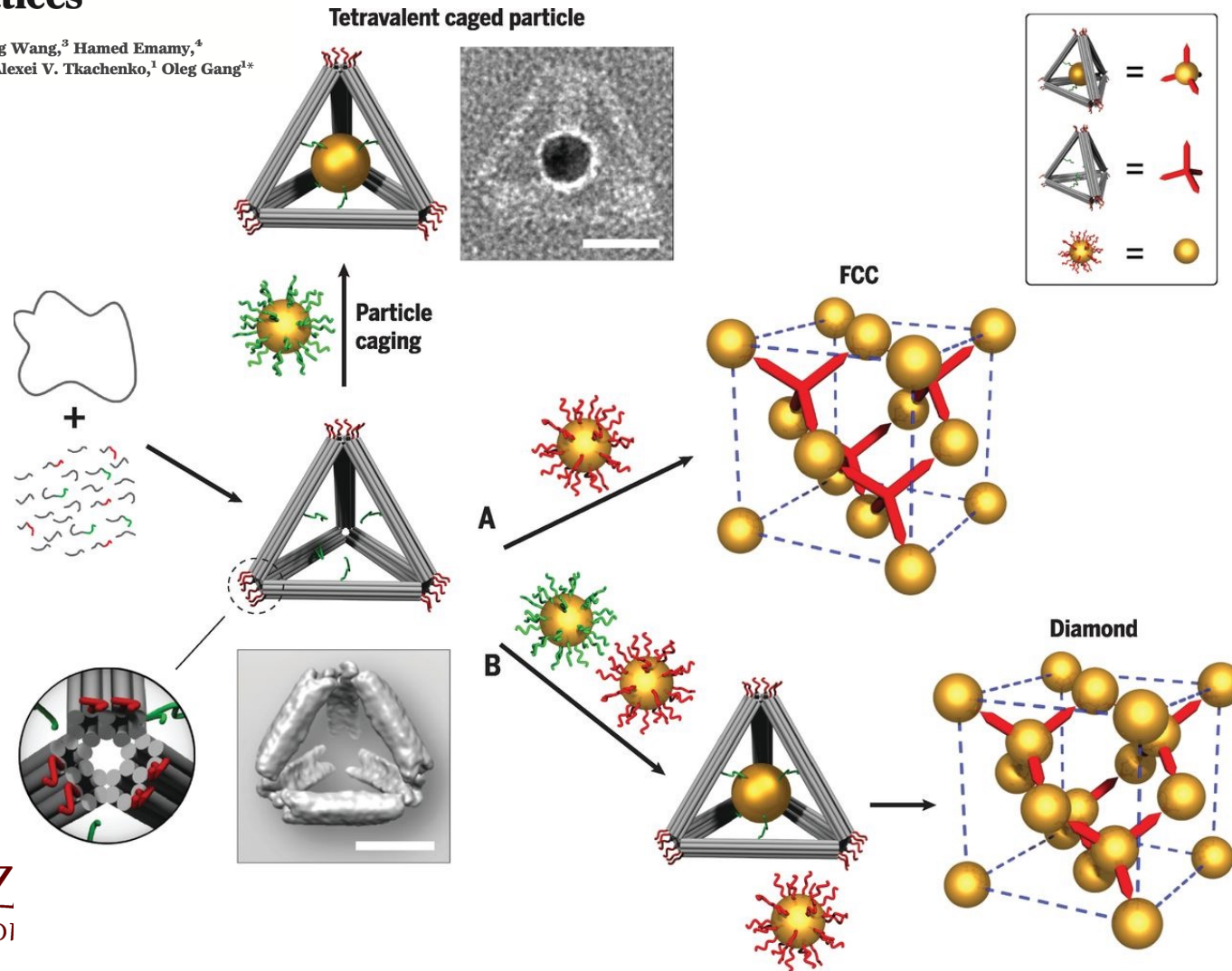
Sanket Kadulkar,¹ Zachary M. Sherman,¹
Venkat Ganesan,¹ and Thomas M. Truskett^{1,2}

¹Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

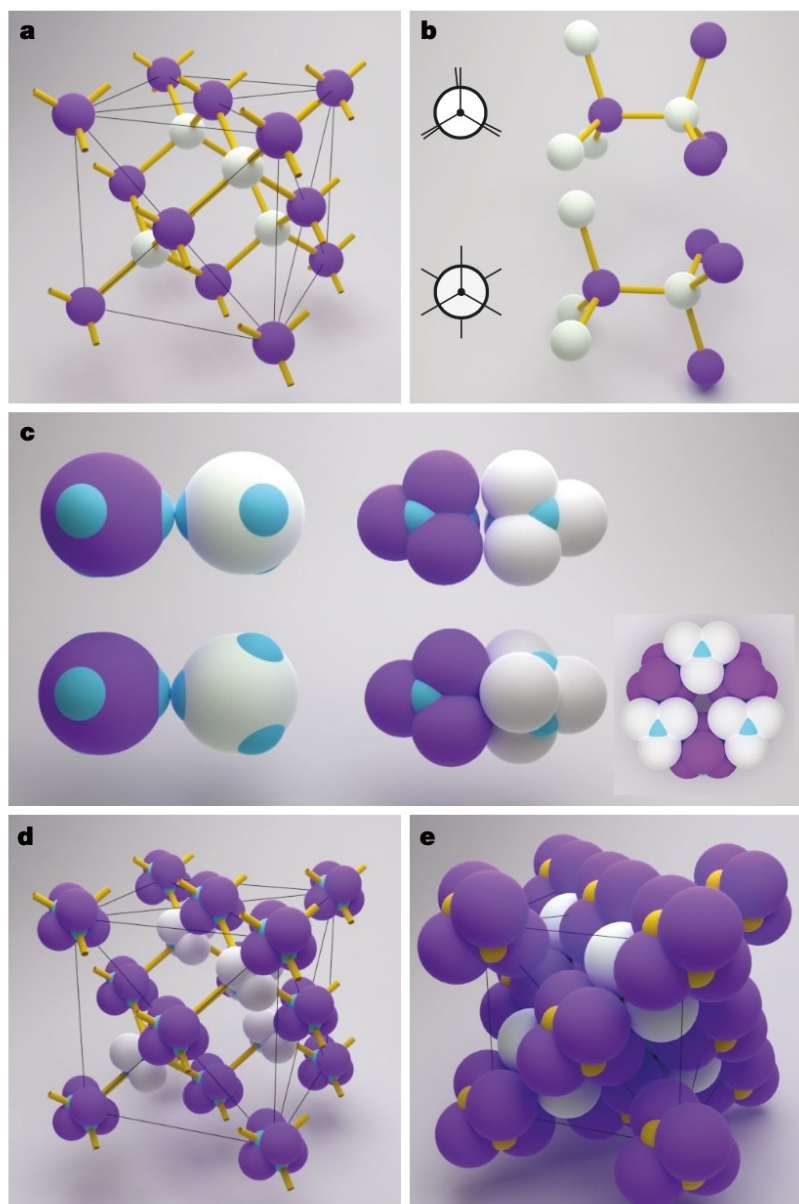
²Department of Chemical Engineering, Princeton University, Princeton, New Jersey 08542, USA

Diamond family of nanoparticle superlattices

Wenyan Liu,¹ Miho Tagawa,² Huolin L. Xin,¹ Tong Wang,³ Hamed Emamy,⁴
Huolin Li,^{3,5} Kevin G. Yager,¹ Francis W. Starr,⁴ Alexei V. Tkachenko,¹ Oleg Gang^{1*}



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Colloidal diamond

<https://doi.org/10.1038/s41586-020-2718-6>

Received: 9 February 2020

Mingxin He^{1,2}, Johnathon P. Gales², Étienne Ducrot^{2,3}, Zhe Gong⁴, Gi-Ra Yi⁵, Stefano Sacanna⁴ & David J. Pine^{1,2}

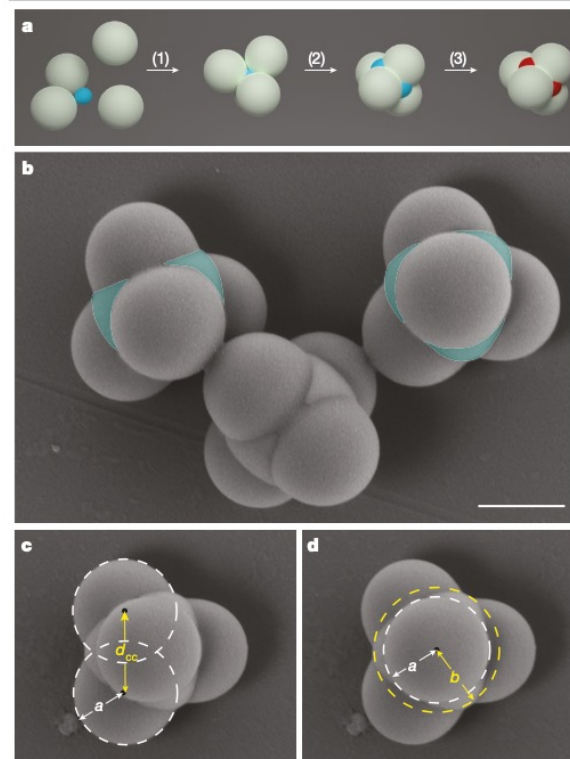


Fig. 2 | Synthesis of compressed tetrahedral patchy clusters. **a**, (1) Aggregation of four polystyrene particles (white) around a smaller oil droplet (blue), followed by (2) controlled deformation of the polystyrene particles with THF, which extrudes the central oil droplet. (3) The THF is then removed, the oil polymerized and coated with DNA to produce solid compressed tetrahedral clusters with DNA-coated patches (red). **b**, Scanning electron microscopy (SEM) image of compressed tetrahedral clusters. Some TPM patches are highlighted in light blue. Scale bar, 1 μm . **c**, The compression ratio $d_{cc}/(2a)$ is defined as the distance between the centres of the spherical lobes divided by

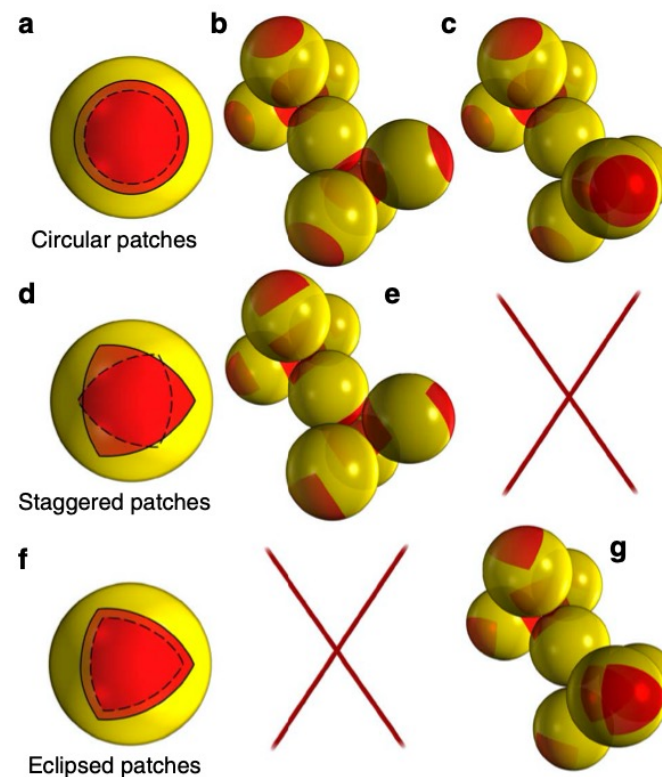
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Received 12 Mar 2012 | Accepted 21 Jun 2012 | Published 24 Jul 2012

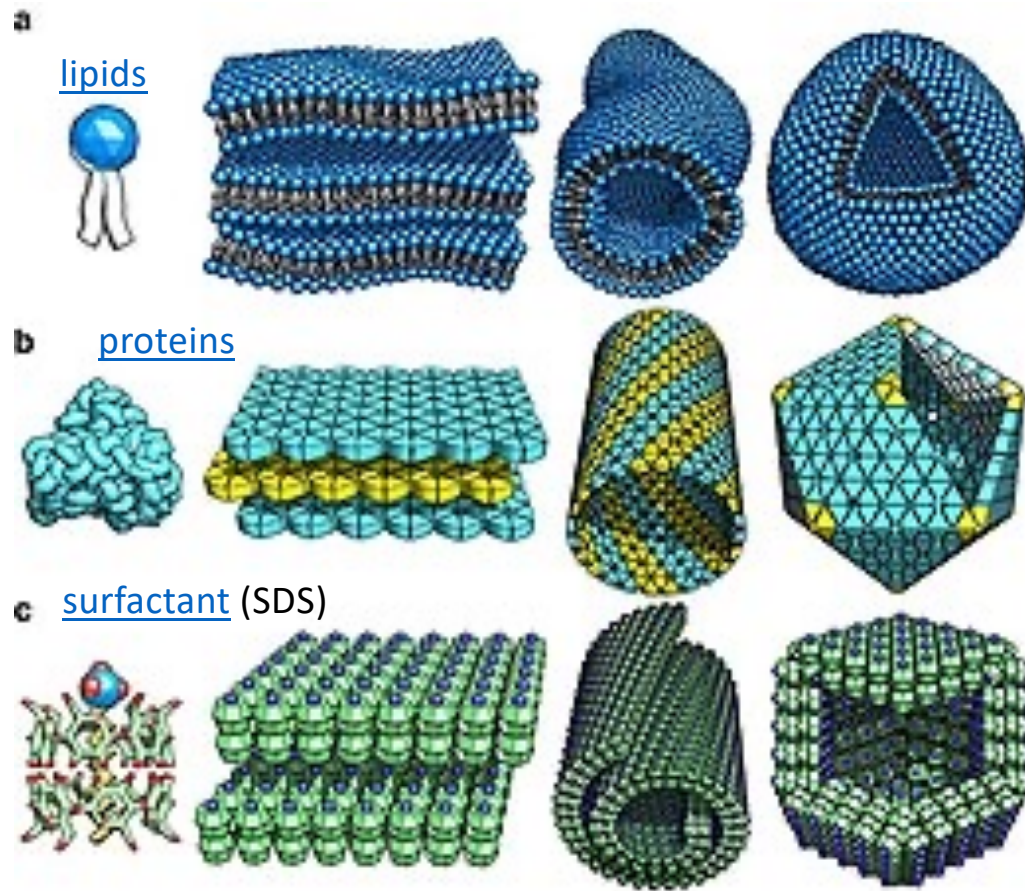
DOI: 10.1038/ncomms1968

Patterning symmetry in the rational design of colloidal crystals

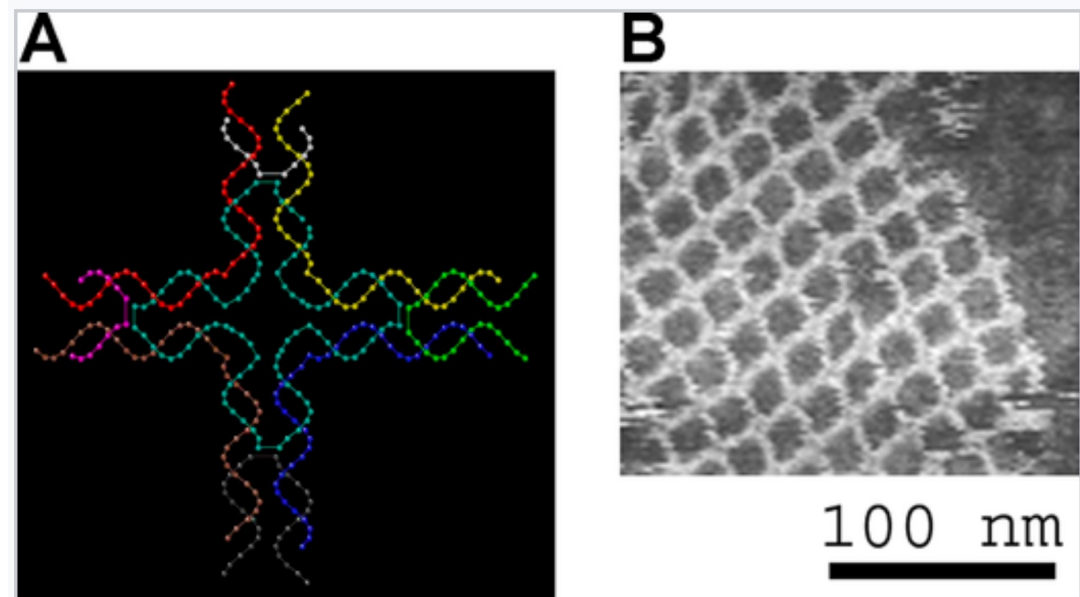
Flavio Romano^{1,*} & Francesco Sciortino^{2,*}



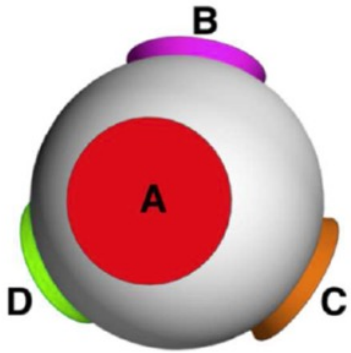
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≡ Self-assembly



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$$\Delta_{\alpha\gamma} = \frac{V_b}{\pi\sigma^3/6} \left(e^{\beta\epsilon_{\alpha\gamma}} - 1 \right)$$

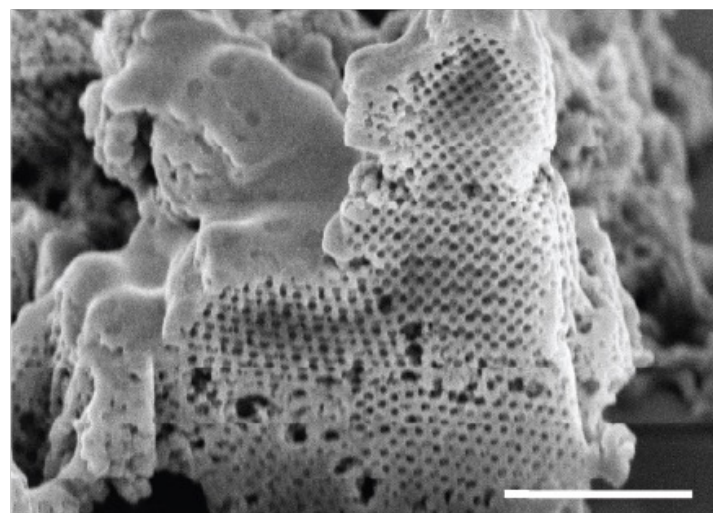
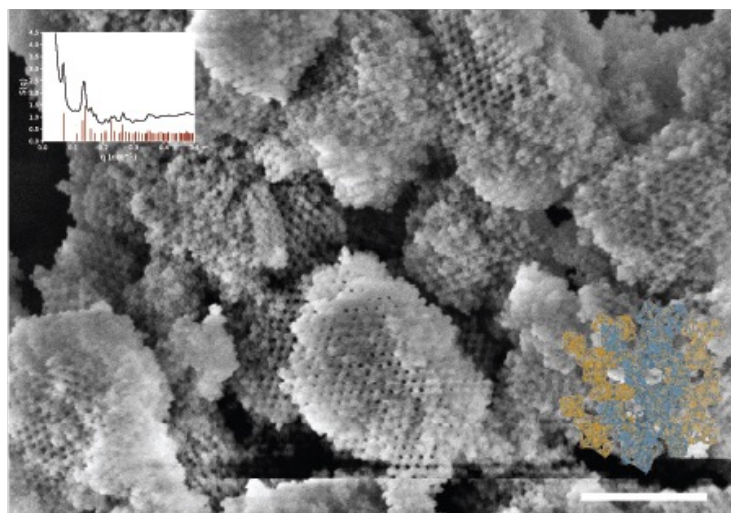
$X_{\alpha}^{(i)}$ = probability that patch α of particle i is not bonded

$$X_{\alpha}^{(i)} = \left[1 + \phi \sum_{j=1, N_s} x^{(j)} \sum_{\gamma \in \Gamma(j)} X_{\gamma}^{(j)} \Delta_{\alpha\gamma} \right]^{-1}$$

(mass action law)

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a**b**